

Denis Jacquemin: Publication list 1995–2025 (as 10/2025)

A Articles in peer-reviewed journals

1. D. Jacquemin, B. Champagne and J. M. André*
Molecular Orbital Expressions for Approximate Uncoupled Hartree-Fock Second Hyperpolarizabilities. A Pariser-Parr-Pople Assessment for Model Polyacetylene Chains
Chem. Phys. (IF=2.053), **197** (1995) 107–127 [doi](#).
2. D. Jacquemin, B. Champagne*, J. M. André and B. Kirtman
Exploratory Pariser-Parr-Pople Investigation of the Static Longitudinal First Hyperpolarizability of Polymethineimine Chains
Chem. Phys. (IF=2.005), **213** (1996) 217–228 [doi](#).
3. D. Jacquemin*, B. Champagne and J. M. André
Electronic First Hyperpolarizability of Polymethineimine Chains with Donor and Acceptor Groups
Synth. Met. (IF=1.256), **80** (1996) 205–210 [doi](#).
4. B. Champagne*, D. Jacquemin, J. M. André and B. Kirtman
Ab Initio Coupled Hartree-Fock Investigation of the Static First Hyperpolarizability of Model All-Trans Polymethineimine Oligomers of Increasing Size
J. Phys. Chem. A (IF=3.392), **101** (1997) 3158–3165 [doi](#).
5. D. Jacquemin*, B. Champagne and J. M. André
Electron Correlation Effects upon the Static (Hyper)polarizabilities of Push-Pull Conjugated Polyenes and Polyynes
Int. J. Quantum Chem. (IF=1.341), **65** (1997) 679–688 [doi](#).
6. D. Jacquemin*, B. Champagne and B. Kirtman
Ab Initio Static Polarizability and First Hyperpolarizability of Model Polymethineimine Chains. 2. Effects of Conformation and of Substitution by Donor/Acceptor End Groups
J. Chem. Phys. (IF=3.247), **107** (1997) 5076–5087 [doi](#).
7. D. Jacquemin*, J. A. Morales, E. Deumens and Y. Öhrn
Electron Nuclear Dynamics of Proton Collisions with Methane at 30 eV
J. Chem. Phys. (IF=3.247), **107** (1997) 6146–6155 [doi](#).
8. D. Jacquemin*, B. Champagne and J. M. André
Ab Initio Band Structure of Polymethineimine Isomers
J. Chem. Phys. (IF=3.147), **108** (1998) 1023–1030 [doi](#).
9. D. Jacquemin*, B. Champagne and J. M. André
Static First Hyperpolarizability of Small All-Trans Polymethineimine Oligomers. Basis Set and Electron Correlation Effects
J. Mol. Struct. (THEOCHEM) (IF=1.048), **425** (1998) 69–79 [doi](#).
10. D. Jacquemin*, B. Champagne and J. M. André
Møller-Plesset Evaluation of the Static First Hyperpolarizability of Polymethineimine
Chem. Phys. Lett. (IF=2.257), **284** (1998) 24–30 [doi](#).
11. B. Champagne*, E. A. Perpète, T. Legrand, D. Jacquemin and J. M. André
Ab Initio Determination of the Vibrational and Electronic First Hyperpolarizabilities of Reference Compounds for Non-Linear Optical (NLO) Applications: 3-Methyl 4-Nitropyridine 1-Oxide (POM) and N-(4-Nitrophenyl)-(L)-Prolinol (NPP)
J. Chem. Soc. Faraday Trans. (IF=1.757), **94** (1998) 1547–1553 [doi](#).
12. D. Jacquemin*, J. M. André and B. Champagne
Long-Range Effects in Optimizing the Geometry of Stereoregular Polymers. I. Formalism
J. Chem. Phys. (IF=3.289), **111** (1999) 5306–5323 [doi](#).
13. D. Jacquemin*, J. M. André and B. Champagne
Long-Range Effects in Optimizing the Geometry of Stereoregular Polymers. II. Hydrogen Fluoride Chains as a Working Example
J. Chem. Phys. (IF=3.289), **111** (1999) 5324–5330 [doi](#).

14. D. Jacquemin and B. Champagne*
Comment on "Calculation of Ab Initio Hyperpolarizabilities of Polymers" [J. Chem. Phys. 110, 2717 (1999)]
J. Chem. Phys. (IF=3.301), **112** (2000) 1616–1617 [doi](#).
15. D. Jacquemin*, B. Champagne and C. Hättig
Correlated Frequency-Dependent Electronic First Hyperpolarizability of Small Push-Pull Conjugated Chains
Chem. Phys. Lett. (IF=2.364), **319** (2000) 327–334 [doi](#).
16. B. Champagne*, E. A. Perpète, D. Jacquemin, S. van Gisbergen, E. V. Baerends, C. Soubra-Ghaoui, K. A. Robins and B. Kirtman
Assessment of Conventional Density Functional Schemes for Computing the Polarizabilities and First Hyperpolarizabilities of Push-Pull π -Conjugated Systems
J. Phys. Chem. A (IF=2.754), **104** (2000) 4755–4763 [doi](#).
17. M. Spassova, T. Kolev, I. Kanev, D. Jacquemin and B. Champagne*
Structure and Nonlinear Electrical Properties of Squaric Acid Derivatives: A Theoretical Study of the Conformation and Deprotonation Effects
J. Mol. Struct. (THEOCHEM) (IF=0.961), **528** (2000) 151–159 [doi](#).
18. E. A. Perpète*, B. Champagne and D. Jacquemin
Electronic and Vibrational First Hyperpolarizability of Polymethineimine
J. Mol. Struct. (THEOCHEM) (IF=0.961), **529** (2000) 65–71 [doi](#).
19. D. Jacquemin* and B. Champagne
Optimizing the Geometry of Stereoregular Polymers. III. Polyynes and the Problem of Basis Set Linear Dependences
Int. J. Quantum Chem. (IF=1.317), **80** (2000) 863–870 [doi](#).
20. T. D. Poulsen*, K. V. Mikkelsen, J. G. Fripiat, D. Jacquemin and B. Champagne
MP2 Correlation Effects upon the Electronic and Vibrational Properties of Polyynes
J. Chem. Phys. (IF=3.147), **114** (2001) 5917–5922 [doi](#).
21. D. Jacquemin*, B. Champagne, E. A. Perpète, J. M. Luis and B. Kirtman
Second-Order Møller-Plesset Study of Optimum Chain Length for Total (Electronic plus Vibrational) $\beta(-\omega_\sigma; \omega_1, \omega_2)$ of a Prototype Push-Pull Polyene
J. Phys. Chem. A (IF=2.630), **105** (2001) 9748–9755 [doi](#).
22. D. Jacquemin*, D. Beljonne, B. Champagne, V. Geskin, J. L. Brédas and J. M. André
Analysis of the Sign Reversal of the Second-Order Molecular Polarizability of Polymethineimine Chains
J. Chem. Phys. (IF=3.147), **115** (2001) 6766–6774 [doi](#).
23. D. Jacquemin* and B. Champagne
Long-Range Effects in Optimizing the Geometry of Stereoregular Polymers–IV: Explicit Determination of the Helical Angle
Int. J. Quantum Chem. (IF=1.249), **85** (2001) 539–545 [doi](#).
24. D. Jacquemin*, E. A. Perpète and B. Champagne
First Hyperpolarizability of H-(BN)N-H Oligomers: Analysis of Geometry, Asymmetry and Delocalization Effects
Phys. Chem. Chem. Phys. (IF=1.838), **4** (2002) 432–440 [doi](#).
25. D. Jacquemin*, J. G. Fripiat and B. Champagne
Convergence of Exchange Lattice Summations in Direct-Space Polymer Calculations
Int. J. Quantum Chem. (IF=1.514), **89** (2002) 452–463 [doi](#).
26. M. Yang, D. Jacquemin and B. Champagne*
Intramolecular Charge Transfer and First-Order Hyperpolarizability of Planar and Twisted Sesquifulvalenes
Phys. Chem. Chem. Phys. (IF=1.838), **4** (2002) 5566–5571 [doi](#).

27. D. Jacquemin*, B. Champagne, J. M. André, E. Deumens and Y. Öhrn
Integral Algorithm and Density Matrix Integration Scheme for Ab Initio Band Structure Calculations on Polymeric Systems
J. Comput. Chem. (IF=2.931), **23** (2002) 1430–1444 [doi](#).
28. D. Jacquemin*, J. M. André and B. Champagne
Analytic Ab Initio Determination of the Elastic Modulus in Stereoregular Polymers. Analytical Integrals Derivatives, Long-Range Effects, Implementation, and Examples
J. Chem. Phys. (IF=2.950), **118** (2003) 373–388 [doi](#).
29. D. Jacquemin*, J. M. André and B. Champagne
Analytic Ab Initio Determination of the IR Intensities in Stereoregular Polymers
J. Chem. Phys. (IF=2.950), **118** (2003) 3956–3965 [doi](#).
30. D. Jacquemin*, B. Champagne and J. M. André
Copolymerization Effects upon the Second-Order NLO Responses of Polyacetylene/Polymethineimine Macromolecules (IF=3.621), **36** (2003) 3980–3985 [doi](#).
31. B. Champagne*, D. Jacquemin, F. L. Gu, Y. Aoki, D. M. Bishop and B. Kirtman
Pseudo Linear-Dependence and Long-Range Interaction on the Polarizability and Hyperpolarizabilities of Stereoregular Polymers
Chem. Phys. Lett. (IF=2.438), **373** (2003) 539–549 [doi](#).
32. D. Jacquemin*
Theoretical Study of Dehydrogenation Effects upon the First Hyperpolarizability of Polyphosphinoborane
J. Phys. Chem. A (IF=2.639), **108** (2004) 500–506 [doi](#).
33. D. Jacquemin*, C. Lambert and E. A. Perpète
Structures and Properties of Polyphosphinoborane: an Oligomeric Theoretical Study
Macromolecules (IF=3.898), **37** (2004) 1009–1015 [doi](#).
34. D. Jacquemin*, O. Quinet, B. Champagne and J. M. André
Second-Order Nonlinear Optical Coefficient of Polyphosphazene-Based Materials: a Theoretical Study
J. Chem. Phys. (IF=3.105), **120** (2004) 9401–9409 [doi](#).
35. D. Jacquemin*, E. A. Perpète and J. M. André
Theoretical Study of the Longitudinal First Hyperpolarizability of Polysilaacetylene
J. Chem. Phys. (IF=3.105), **120** (2004) 10317–10327 [doi](#).
36. D. Jacquemin*, J. Preat, M. Charlot, V. Wathélet, J. M. André and E. A. Perpète
Theoretical Investigation of Substituted Anthraquinone Dyes
J. Chem. Phys. (IF=3.105), **121** (2004) 1736–1743 [doi](#).
37. D. Jacquemin*, V. Wathélet and E. A. Perpète
Effects of Chain Substitution on the Structures and Properties of Polyphosphinoborane
Macromolecules (IF=3.898), **37** (2004) 5040–5046 [doi](#).
38. D. Jacquemin*, J. M. André and E. A. Perpète
Geometry, Dipole Moment, Polarizability and First Hyperpolarizability of Polymethineimine: an Assessment of Electron Correlation Contributions
J. Chem. Phys. (IF=3.105), **121** (2004) 4389–4396 [doi](#).
39. D. Jacquemin*
First Hyperpolarizability of Polyaminoborane and Polyiminoborane Oligomers
J. Phys. Chem. A (IF=2.639), **108** (2004) 9260–9266 [doi](#).
40. D. Jacquemin*, E. A. Perpète, V. Wathélet and J. M. André
An Ab Initio Investigation of the Structures and Properties of Polyaminoborane
J. Phys. Chem. A (IF=2.639), **108** (2004) 9616–9624 [doi](#).
41. D. Jacquemin*, X. Assfeld and E. A. Perpète
Solvent Effects on the Geometry and First Hyperpolarizability of Polymethineimine
J. Mol. Struct. (THEOCHEM) (IF=1.007), **710** (2004) 13–17 [doi](#).

42. M. Medved', J. Noga, D. Jacquemin and E. A. Perpète
Longitudinal NLO Properties of C₂H₂, HCCF, and C₂F₂: Electron Correlation and Vibration Effects
Int. J. Quantum Chem. (IF=1.192), **102** (2005) 209–223 [doi](#).
43. D. Jacquemin*
Linear and NonLinear Optics Properties of Polyphosphazene/Polynitrile Copolymers
J. Chem. Theory Comput. (IF=NA, 2006 FI=3.627), **1** (2005) 307–314 [doi](#).
44. D. Jacquemin, E. A. Perpète, I. Ciofini and C. Adamo*
Assessment of Recently-Developed Density Functional Approaches for the Evaluation of the Bond Length Alternation in Polyacetylene
Chem. Phys. Lett. (IF=2.438), **405** (2005) 376–381 [doi](#).
45. D. Jacquemin*, J. Preat, V. Wathelet, J. M. André and E. A. Perpète
Substitution Effects on the Visible Spectra of 1,4-diNHP-9,10-Anthraquinone
Chem. Phys. Lett. (IF=2.438), **405** (2005) 429–433 [doi](#).
46. D. Jacquemin*, M. Medved' and E. A. Perpète
Linear Phosphorus-Boron Chains: a Model System with Huge Electronic First Hyperpolarizability
Int. J. Quantum Chem. (IF=1.192), **103** (2005) 226–234 [doi](#).
47. D. Y. Zhang, C. Pouchan, D. Jacquemin* and E. A. Perpète
Ab Initio Studies of the Static Electronic First Hyperpolarizability of Polysilanenitrile
Chem. Phys. Lett. (IF=2.438), **408** (2005) 226–231 [doi](#).
48. D. Jacquemin*, A. Femenias, H. Chermette*, J. M. André* and E. A. Perpète*
A Second-Order Møller-Plesset Evaluation of the Bond Length Alternation of Linear Oligomers
J. Phys. Chem. A (IF=2.898), **109** (2005) 5734–5741 [doi](#).
49. D. Jacquemin* and E. A. Perpète
Ab Initio Assessment of the First Hyperpolarizability of Saturated and Unsaturated Polyaminoborane / Polyphosphinoborane Copolymers
J. Phys. Chem. A (IF=2.898), **109** (2005) 6380–6386 [doi](#).
50. D. Jacquemin*, J. Preat and E. A. Perpète
A TD-DFT Study of the Absorption Spectra of Fast Dye Salts
Chem. Phys. Lett. (IF=2.438), **410** (2005) 254–259 [doi](#).
51. D. Jacquemin*, J. Preat, V. Wathelet and E. A. Perpète
Theoretical Investigation of the Absorption Spectrum of Thioindigo Dyes
J. Mol. Struct. (THEOCHEM) (IF=1.045), **731** (2005) 67–72 [doi](#).
52. J. Preat*, D. Jacquemin and E. A. Perpète
Theoretical Investigation of the UV Spectra of Coumarin Derivatives
Chem. Phys. Lett. (IF=2.438), **415** (2005) 20–24 [doi](#).
53. D. Jacquemin*, E. A. Perpète and J. M. André
NLO Response of Polymethineimine and Polymethineimine/Polyacetylene Conformers: Assessment of Electron Correlation Effects
Int. J. Quantum Chem. (IF=1.192), **105** (2005) 553–563 [doi](#).
54. D. Y. Zhang, C. Pouchan, E. A. Perpète and D. Jacquemin*
Ab Initio Prediction of Extremely Large First Hyperpolarizability of Polyphosphaacetylene and Polyphosphasilyne
Chem. Phys. Lett. (IF=2.438), **416** (2005) 277–281 [doi](#).
55. L. Briquet, D. P. Vercauteren, E. A. Perpète and D. Jacquemin*
Is Solvated Trans-Azobenzene Twisted or Planar?
Chem. Phys. Lett. (IF=2.462), **417** (2006) 190–195 [doi](#).
56. D. Jacquemin*, J. Preat, V. Wathelet, M. Fontaine and E. A. Perpète
Thioindigo Dyes: Highly Accurate Visible Spectra with TD-DFT
J. Am. Chem. Soc. (IF=7.696), **128** (2006) 2072–2083 [doi](#).

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57. D. Jacquemin*, J. Preat, V. Wathelet and E. A. Perpète
Substitution and Chemical Environment Effects on the Absorption Spectrum of Indigo
J. Chem. Phys. (IF=3.166), **124** (2006) 074104 (12 p.) [doi](#).
58. D. Jacquemin* and E. A. Perpète
The $n \rightarrow \pi^$ Transition in Nitroso Compounds: a TD-DFT Study*
Chem. Phys. Lett. (IF=2.462), **420** (2006) 529–533 [doi](#).
59. E. A. Perpète, V. Wathelet, J. Preat, C. Lambert and D. Jacquemin*
Toward a Theoretical Quantitative Estimation of the $\lambda_{\max}$ of Anthraquinones-Based Dyes
J. Chem. Theory Comput. (IF=3.627), **2** (2006) 434–440 [doi](#).
60. D. Jacquemin, E. A. Perpète, G. Scalmani, M. J. Frisch, I. Ciofini and C. Adamo*
Absorption and Emission Spectra in Gas-Phase and Solution Using TD-DFT: Formaldehyde and Benzene as Case Studies
Chem. Phys. Lett. (IF=2.462), **421** (2006) 272–276 [doi](#).
61. V. Wathelet, J. Preat, M. Bouhy, M. Fontaine, E. A. Perpète, J. M. André and D. Jacquemin*
Assessment of PBE0 for Evaluating the Absorption Spectra of Carbonyl Molecules
Int. J. Quantum Chem. (IF=1.182), **106** (2006) 1853–1859 [doi](#).
62. E. A. Perpète, J. Preat, J. M. André and D. Jacquemin*
An Ab Initio Study of the Absorption Spectra of Indirubin, Isoindigo, and Related Compounds
J. Phys. Chem. A (IF=3.047), **110** (2006) 5629–5635 [doi](#).
63. D. Jacquemin*, A. Femenias, H. Chermette, I. Ciofini, C. Adamo, J. M. André, and E. A. Perpète
Assessment of Several Hybrid DFT Functionals for the Evaluation of Bond Length Alternation of Increasingly Long Oligomers
J. Phys. Chem. A (IF=3.047), **110** (2006) 5952–5959 [doi](#).
64. D. Jacquemin*, M. Bouhy and E. A. Perpète
Excitation Spectra of Nitro-Diphenylaniline: Accurate Time-Dependent Density Functional Theory Predictions for Charge-Transfer Dyes
J. Chem. Phys. (IF=3.166), **124** (2006) 204321 (9 p.) [doi](#).
65. J. Preat*, D. Jacquemin, V. Wathelet, J. M. André and E. A. Perpète
TD-DFT Investigation of the UV Spectra of Pyranone Derivatives
J. Phys. Chem. A (IF=3.047), **110** (2006) 8144–8150 [doi](#).
66. D. Jacquemin*, V. Wathelet and E. A. Perpète
Ab Initio Investigation of the $n \rightarrow \pi^$ Transitions in Thiocarbonyl Dyes*
J. Phys. Chem. A (IF=3.047), **110** (2006) 9145–9152 [doi](#).
67. D. Jacquemin* and E. A. Perpète
Ab Initio Calculations of the Colour of Closed-Ring Diarylethenes: TD-DFT Estimates for Molecular Switches
Chem. Phys. Lett. (IF=2.462), **429** (2006) 147–152 [doi](#).
68. D. Jacquemin*, J. Preat, V. Wathelet and E. A. Perpète
Time-Dependent Density Functional Theory Determination of the Absorption Spectra of Naphthoquinones
Chem. Phys. (IF=1.984), **328** (2006) 324–332 [doi](#).
69. J. de Ruyck*, J. Preat, E. A. Perpète, D. Jacquemin and J. Wouters
2,6-Dihydroxyanthraquinone, an Isomer of Well-Known Alizarin Dye
Acta Cryst. E (IF=0.567), **62** (2006) o4503–o4505 [doi](#).
70. D. Jacquemin*, E. A. Perpète, G. Scalmani, M. J. Frisch, X. Assfeld, I. Ciofini and C. Adamo*
TD-DFT Investigation of the Absorption, Fluorescence, and Phosphorescence Spectra of Solvated Coumarins
J. Chem. Phys. (IF=3.166), **125** (2006) 164324 (11 p.) [doi](#).

71. J. Preat*, D. Jacquemin and E. A. Perpète
A TD-DFT Investigation of the Visible Spectra of Fluoro-Anthraquinones
Dyes Pigm. (IF=2.796), **72** (2007) 185–191 [doi](#).
72. J. Preat*, P. F. Loos, X. Assfeld, D. Jacquemin and E. A. Perpète
DFT and TD-DFT Investigation of IR and UV Spectra of Solvated Molecules: Comparison of two SCRF Continuum Models
Int. J. Quantum Chem. (IF=1.368), **107** (2007) 574–585 [doi](#).
73. D. Jacquemin*, E. A. Perpète, H. Chermette, I. Ciofini and C. Adamo
Comparison of Theoretical Approaches for Computing the Bond Length Alternation of Polymethineimine
Chem. Phys. (IF=1.805), **332** (2007) 79–85 [doi](#).
74. D. Jacquemin* and E. A. Perpète
On the Basis Set Convergence of TD-DFT Oscillator Strengths: Dinitrophenylhydrazones as a Case Study
J. Mol. Struct. (THEOCHEM) (IF=1.112), **804** (2007) 31–34 [doi](#).
75. L. Briquet, D. P. Vercauteren, J. M. André, E. A. Perpète and D. Jacquemin*
On the Geometries and UV/Vis Spectra of Substituted Trans-Azobenzenes
Chem. Phys. Lett. (IF=2.207), **435** (2007) 257–262 [doi](#).
76. E. A. Perpète and D. Jacquemin*
An Ab Initio Scheme for Quantitative Predictions of the Visible Spectra of Diarylethenes
J. PhotoChem. PhotoBiol. A: Chem. (IF=1.911), **187** (2007) 40–44 [doi](#).
77. A. D. Laurent, J. M. André, E. A. Perpète and D. Jacquemin*
Hemi-Indigo Photochroms: a Theoretical Investigation
Chem. Phys. Lett. (IF=2.207), **436** (2007) 84–88 [doi](#).
78. D. Jacquemin, X. Assfeld, J. Preat and E. A. Perpète*
Comparison of Theoretical Approaches for Predicting the UV/Vis Spectra of Anthraquinones
Mol. Phys. (IF=1.568), **105** (2007) 325–331 [doi](#).
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Hottest Articles 79. J. Preat*, P. F. Loos, X. Assfeld, D. Jacquemin and E. A. Perpète
A TD-DFT Investigation of UV Spectra of Pyranoidic Dyes: A NCM vs PCM Comparison
J. Mol. Struct. (THEOCHEM) (IF=1.112), **808** (2007) 85–91 [doi](#).
- Top 25**
Hottest Articles 80. D. Jacquemin*, E. A. Perpète, X. Assfeld, G. Scalmani, M. J. Frisch and C. Adamo*
The Geometries, Absorption and Fluorescence Wavelengths of Solvated Fluorescent Coumarins: a CIS and TD-DFT Comparative Study
Chem. Phys. Lett. (IF=2.207), **438** (2007) 208–212 [doi](#).
- Top 20** 81. D. Jacquemin*, E. A. Perpète, G. Scalmani, M. J. Frisch, R. Kobayashi and C. Adamo*
Assessment of the Efficiency of Long-Range Corrected Functionals for Some Properties of Large Compounds
J. Chem. Phys. (IF=3.044), **126** (2007) 144105 (12 p.) [doi](#).
82. D. Jacquemin*, V. Wathelet, J. Preat and E. A. Perpète
Ab Initio Tools for the Accurate Prediction of the Visible Spectra of Anthraquinones
Spectrochim. Acta A (IF=1.511), **67** (2007) 334–341 [doi](#).
83. E. A. Perpète and D. Jacquemin*
Ab Initio Investigation of the Solvent and Electron Correlation Effects on the Geometries and Static First Hyperpolarizabilities of Push-Pull Oligomers
Int. J. Quantum Chem. (IF=1.368), **107** (2007) 2066–2074 [doi](#).
84. D. Jacquemin*, E. A. Perpète, M. Medved', G. Scalmani, M. J. Frisch, R. Kobayashi and C. Adamo*
First Hyperpolarizability of Polymethineimine with Long-Range Corrected Functionals
J. Chem. Phys. (IF=3.044), **126** (2007) 191108 (4 p.) [doi](#).

85. J. Preat*, D. Jacquemin, V. Wathelet, J. M. André and E. A. Perpète
Towards the Understanding of the Chromatic Behaviour of Triphenylmethane Derivatives
Chem. Phys. (IF=1.805), **335** (2007) 177–186 [doi](#).
86. E. A. Perpète, F. Maurel and D. Jacquemin*
TD-DFT Investigation of Diarylethene Dyes with Cyclopentene, Dihydrothiophene, and Dihydropyrrole Bridges
J. Phys. Chem. A. (IF=2.918), **111** (2007) 5528–5535 [doi](#).
87. C. Michaux, J. Wouters, D. Jacquemin* and E. A. Perpète
A Theoretical Investigation of the Hydrated Glycine Cation Energetics and Structures
Chem. Phys. Lett. (IF=2.207), **445** (2007) 57–61 [doi](#).
- Top 20** 88. D. Jacquemin*, E. A. Perpète, O. A. Vydrov, G. E. Scuseria and C. Adamo*
Assessment of Long-Range Corrected Functionals Performance for $n \rightarrow \pi^$ Transitions in Organic Dyes*
J. Chem. Phys. (IF=3.044), **127** (2007) 094102 (6 p.) [doi](#).
89. M. Medved', J. Noga, D. Jacquemin, X. Assfeld and E. A. Perpète
NLO Responses of Small Polymethineimine Oligomers: a CCSD(T) Study
J. Mol. Struct. (THEOCHEM) (IF=1.112), **821** (2007) 160–165 [doi](#).
90. A. D. Laurent, J. M. André, E. A. Perpète and D. Jacquemin*
Photochromic Properties of Dithienylazoles and Other Conjugated Diarylethenes
J. PhotoChem. PhotoBiol. A: Chem. (IF=1.911), **192** (2007) 211–219 [doi](#).
- Top 25** 91. D. Jacquemin*, E. A. Perpète, G. Scalmani, M. J. Frisch, I. Ciofini and C. Adamo*
Fluorescence of 1,8-Naphthalimide: a PCM-TD-DFT Investigation
Hottest Articles Chem. Phys. Lett. (IF=2.207), **448** (2007) 3–6 [doi](#).
92. M. Medved', M. Stachova, D. Jacquemin, J. M. André and E. A. Perpète
A Generalized Romberg Differentiation Procedure
J. Mol. Struct. (THEOCHEM) (IF=1.112), **847** (2007) 39–46 [doi](#).
93. E. A. Perpète, C. Lambert, V. Wathelet, J. Preat and D. Jacquemin*
Ab Initio Studies of the $\lambda_{\max}$ of Naphthoquinones Dyes
Spectrochim. Acta A (IF=1.511), **68** (2007) 1326–1333 [doi](#).
94. D. Jacquemin* and E. A. Perpète
Evaluation Ab Initio de la Couleur de Diaryléthènes Présentant un Pont Maléimide
Comptes Rendus Chimie (IF=1.305), **10** (2007) 1227–1233 [doi](#).
95. J. de Ruyck, M. Famerée, J. Wouters, E. A. Perpète, J. Preat and D. Jacquemin*
Towards the Understanding of the Absorption Spectra of NAD(P)H/NAD(P)⁺ as a Common Indicator of Dehydrogenase Enzymatic Activity
Chem. Phys. Lett. (IF=2.207), **450** (2007) 119–122 [doi](#).
96. J. Preat, C. Michaux, A. Lewalle, E. A. Perpète and D. Jacquemin*
Delocalisation in Conjugated Triazene Chromophores: Insights from Theory
Chem. Phys. Lett. (IF=2.169), **451** (2008) 37–42 [doi](#).
97. J. Preat*, D. Jacquemin and E. A. Perpète
Tayloring Standard TDDFT Approaches for Computing UV/Vis Transitions in Thiocarbonyl Chromophores
Int. J. Quantum Chem. (IF=1.317), **108** (2008) 768–773 [doi](#).
98. D. Jacquemin*, E. A. Perpète, G. E. Scuseria, I. Ciofini and C. Adamo*
TD-DFT Performance for the Visible Absorption Spectra of Organic Dyes: Conventional versus Long-Range Hybrids
THE MOST J. Chem. Theory Comput. (IF=4.274), **4** (2008) 123–135 [doi](#).
HIGHLY CITED
99. D. Jacquemin, E. A. Perpète, I. Ciofini and C. Adamo*
A Fast and Reliable Theoretical Determination of pK_a^ for Photoacids*
THE MOST J. Phys. Chem. A. (IF=2.871), **112** (2008) 794–796 [doi](#).



100. C. Michaux, J. Wouters, E. A. Perpète and D. Jacquemin*
Microhydration of Protonated Glycine: an Ab Initio Family Tree
J. Phys. Chem. B. (IF=4.189), **112** (2008) 2430–2438 [doi](#).
101. D. Jacquemin*, E. A. Perpète, I. Ciofini and C. Adamo
Revisiting the Relationship Between the Bond Length Alternation and the First Hyperpolarizability with Range-Separated Hybrid Functionals
J. Comput. Chem. (IF=3.390), **29** (2008) 921–925 [doi](#).
102. J. Preat*, D. Jacquemin, D. P. Vercauteren and E. A. Perpète
A Quantitative Prediction of the Electronic Spectra of Thiocarbonyl Chromophore: TD-DFT vs SAC-CI
Theor. Chem. Acc. (IF=2.370), **119** (2008) 463–468 [doi](#).
103. E. A. Perpète, D. Jacquemin, C. Adamo* and G. E. Scuseria
Revisiting the Nonlinear Optical Properties of Polybutatriene and Polydiacetylene with Density Functional Theory
Chem. Phys. Lett. (IF=2.169), **456** (2008) 101–104 [doi](#).
104. P. F. Loos*, J. Preat, A. D. Laurent, C. Michaux, D. Jacquemin, E. A. Perpète and X. Assfeld
Theoretical Investigation of the Geometries and UV/Vis Spectra of Poly(L-Glutamic Acid) Featuring Photochromic Azobenzene Side Chain
J. Chem. Theory Comput. (IF=4.274), **4** (2008) 637–645 [doi](#).
105. D. Jacquemin*, A. Lewalle and E. A. Perpète
Modelling the Acidochromism of Pyridylazulenes
Chem. Phys. Lett. (IF=2.169), **457** (2008) 91–95 [doi](#).
106. D. Jacquemin*, E. A. Perpète, I. Ciofini and C. Adamo*
On the TD-DFT UV/Vis Spectra Accuracy: the Azoalkanes
Theor. Chem. Acc. (IF=2.370), **120** (2008) 405–410 [doi](#).
107. C. Michaux, J. Wouters, E. A. Perpète and D. Jacquemin*
Stepwise Hydration of Protonated Proline
J. Phys. Chem. B (IF=4.189), **112** (2008) 7702–7705 [doi](#).
108. D. Jacquemin*, E. A. Perpète and C. Adamo*
Modelling the UV/Visible Spectrum of Tetrakis(Phenylethynyl)Benzene
J. Mol. Struct. (THEOCHEM) (IF=1.167), **863** (2008) 123–127 [doi](#).
109. C. Michaux, J. Wouters, E. A. Perpète and D. Jacquemin*
Modelling the Microhydration of Protonated Alanine
J. Phys. Chem. B (IF=4.189), **112** (2008) 9896–9902 [doi](#).
110. F. Maurel, A. Perrier, E. A. Perpète and D. Jacquemin*
A Theoretical Study of the Perfluoro-Diarylethenes Electronic Spectra
J. PhotoChem. PhotoBiol. A: Chem. (IF=2.362), **199** (2008) 211–223 [doi](#).
111. J. M. André*, D. Jacquemin, E. A. Perpète, D. P. Vercauteren and V. Wathelet¹
Assessment of the Accuracy of TD-DFT Absorption Spectra: Substituted Benzenes
Coll. Czech Chem. Commun. (IF=0.784), **73** (2008) 898–908 [doi](#).
112. D. Jacquemin*, E. A. Perpète, G. E. Scuseria, I. Ciofini and C. Adamo*
Extensive TD-DFT Investigation of the First Electronic Transition in Substituted Azobenzenes
Chem. Phys. Lett. (IF=2.169), **465** (2008) 226–229 [doi](#).
113. J. Casanovas, D. Jacquemin*, E. A. Perpète and C. Alemán*
Fluorescein Isothiocyanate: Molecular Characterization using Theoretical Calculations
Chem. Phys. (IF=1.961), **354** (2008) 155–161 [doi](#).

¹Alphabetical order list.

114. J. Preat*, D. Jacquemin, J. Burton, D. P. Vercauteren and E. A. Perpète
Quantitative Evaluation of Solvation and Packing Effects on the Visible Absorption Spectra of Anthraquinone Derivatives
Dyes Pigm. (IF=2.855), **81** (2009) 97–102 [doi](#).
115. D. Jacquemin*, E. A. Perpète, A. D. Laurent, X. Assfeld and C. Adamo*
Spectral Properties of Self-Assembled Squaraine-Tetralactam: a Theoretical Assessment
Phys. Chem. Chem. Phys. (IF=4.116), **11** (2009) 1258–1262 [doi](#).
116. D. Jacquemin*, E. A. Perpète, I. Ciofini and C. Adamo*
Accurate Simulation of Optical Properties in Dyes
Acc. Chem. Res. (IF=18.203), **42** (2009) 326–334 [doi](#).
117. C. Michaux, J. Wouters, E. A. Perpète and D. Jacquemin*
Ab Initio Investigation of the Hydration of Deprotonated Amino Acids
J. Am. Soc. Mass. Spectr. (IF=3.391), **20** (2009) 632–638 [doi](#).
118. J. Preat*, A. D. Laurent, C. Michaux, E. A. Perpète and D. Jacquemin
Impact of Tautomers on the Absorption Spectra of Neutral and Anionic Alizarin and Quinizarin Dyes
J. Mol. Struct. (THEOCHEM) (IF=1.216), **901** (2009) 24–30 [doi](#).
119. M. Medved'*, S. Budzak, D. Jacquemin and E. A. Perpète
Enhancement of the Second-Order NLO Responses of Boron-Nitrogen Oligomers by Copolymerization with Polyynes
J. Mol. Struct. (THEOCHEM) (IF=1.216), **901** (2009) 194–201 [doi](#).
120. J. P. Cerón-Carrasco*, A. Requena, C. Michaux, E. A. Perpète and D. Jacquemin
Effects of Hydration on the Proton Transfer Mechanism in the Adenine-Thymine Base Pair
J. Phys. Chem. A (IF=2.899), **113** (2009) 7892–7898 [doi](#).
121. P. Vandurm, C. Cauvin, J. Wouters, E. A. Perpète and D. Jacquemin*
Electronic Transitions of Neutral and Anionic Quinolinone HIV-1 Integrase Inhibitor: Joint Theory/Experiment Investigation
Chem. Phys. Lett. (IF=2.291), **478** (2009) 243–248 [doi](#).
122. D. Jacquemin*, V. Wathélet, E. A. Perpète and C. Adamo*
Extensive TD-DFT Benchmark: Singlet-Excited States of Organic Molecules
J. Chem. Theory Comput. (IF=4.804), **5** (2009) 2420–2435 [doi](#).
123. J. Preat*, C. Michaux, D. Jacquemin and E. A. Perpète
Enhanced Efficiency of Organic Dye-Sensitized Solar Cells: Triphenylamine Derivatives
J. Phys. Chem. C (IF=4.224), **113** (2009) 16821–16833 [doi](#).
124. J. P. Cerón-Carrasco*, A. Requena, A. Zuniga, C. Michaux, E. A. Perpète and D. Jacquemin
Intermolecular Proton Transfer in Microhydrated Guanine-Cytosine Base Pairs: a New Mechanism for Spontaneous Mutation in DNA
J. Phys. Chem. A (IF=2.899), **113** (2009) 10549–10556 [doi](#).
125. D. Jacquemin*, A. D. Laurent, E. A. Perpète and J. M. André*
An Ab Initio Simulation of the UV/Visible Spectra of N-Benzylideneaniline Dyes
Int. J. Quantum Chem. (IF=1.315), **109** (2009) 3506–3515 [doi](#).
126. E. A. Perpète and D. Jacquemin*
TD-DFT Benchmark for Indigoïd Dyes
J. Mol. Struct. (THEOCHEM) (IF=1.216), **914** (2009) 100–105 [doi](#).
127. A. Perrier*, F. Maurel, E. A. Perpète, V. Wathélet and D. Jacquemin*
Spectral Properties of Spirooxazine Photochromes: TD-DFT Insights
J. Phys. Chem. A (IF=2.899), **113** (2009) 13004–13012 [doi](#).
128. J. P. Cerón-Carrasco*, A. Requena, E. A. Perpète, C. Michaux and D. Jacquemin
Double Proton Transfer Mechanism in the Adenine-Uracil Base Pair and Spontaneous Mutation in RNA Duplex
Chem. Phys. Lett. (IF=2.291), **484** (2009) 64–68 [doi](#).



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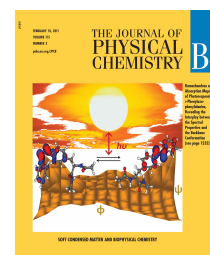
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Ab Initio Investigation of the Electronic Properties of Coupled Dithienylethenes
J. Phys. Chem. Lett. (IF=6.213), **1** (2010) 434–438 [doi](#).
130. A. D. Laurent*, X. Assfeld, D. Jacquemin, J. M. André and E. A. Perpète
Substitution Effects on the Optical Spectra of Diarylethene Photochroms: Ab Initio Insights
Mol. Simul. (IF=1.215), **36** (2010) 74–78 [doi](#).
131. G. Fayet, D. Jacquemin*, V. Wathelet, E. A. Perpète, P. Rotureau and C. Adamo*
Excited-State Properties from Ground-State DFT Descriptors: a QSPR Approach for Dyes
J. Mol. Graph. Model. (IF=2.033), **28** (2010) 465–471 [doi](#).
132. D. Jacquemin*, C. Michaux, E. A. Perpète, F. Maurel and A. Perrier
Photochromic Molecular Wires: Insights from Theory
Chem. Phys. Lett. (IF=2.280), **488** (2010) 193–197 [doi](#).
- Most Read Articles**
HIGHLY CITED 133. D. Jacquemin*, E. A. Perpète, I. Ciofini and C. Adamo*
Assessment of Functionals for TD-DFT Calculations of Singlet-Triplet Transitions
J. Chem. Theory Comput. (IF=5.138), **6** (2010) 1532–1537 [doi](#).
134. D. Jacquemin*, E. A. Perpète, F. Maurel and A. Perrier*
Doubly Closing or not ? Theoretical Analysis for Coupled Photochromes
J. Phys. Chem. C (IF=4.520), **114** (2010) 9489–9497 [doi](#).
- Top 25**
Hottest Articles 135. D. Jacquemin*, E. A. Perpète, G. Scalmani, I. Ciofini, C. Peltier and C. Adamo*
Absorption and Emission Spectra of 1,8-Naphthalimide Fluorophores: a PCM-TD-DFT Investigation
Chem. Phys. (IF=2.017), **372** (2010) 61–66 [doi](#).
136. D. Jacquemin*, C. Peltier and I. Ciofini*
Visible Spectrum of Naphthazarin Investigated through Time-Dependent Density Functional Theory
Chem. Phys. Lett. (IF=2.280), **493** (2010) 67–71 [doi](#).
137. D. Jacquemin*, E. A. Perpète, F. Maurel and A. Perrier*
Simulation of the Properties of a Photochromic Triad
J. Phys. Chem. Lett. (IF=6.213), **1** (2010) 2104–2108 [doi](#).
- Top Ten** 138. J. Preat*, D. Jacquemin and E. A. Perpète
Towards New Efficient Dyes Sensitised Solar Cells
Energy Environ. Sci. (IF=9.446), Perspective Article, **3** (2010) 891–904 [doi](#).
139. D. Jacquemin*, J. Preat, E. A. Perpète and C. Adamo
Absorption Spectra of Recently-Synthesised Organic Dyes: a TD-DFT Study
Int. J. Quantum Chem. (IF=1.302), **110** (2010) 2121–2129 [doi](#).
140. J. Preat*, D. Jacquemin and E. A. Perpète
A UV/Vis Spectra Investigation of pH-Sensitive Dyes using Time-Dependent Density Functional Theory
Int. J. Quantum Chem. (IF=1.302), **110** (2010) 2147–2154 [doi](#).
- Most Read Articles**
HIGHLY CITED 141. D. Jacquemin*, E. A. Perpète, I. Ciofini, C. Adamo*, R. Valero, Y. Zhao and D. G. Truhlar
On the Performances of the M06 Family of Density Functionals for Electronic Excitation Energies
J. Chem. Theory Comput. (IF=5.138), **6** (2010) 2071–2085 [doi](#).
142. J. Preat*, D. Jacquemin and E. A. Perpète
Design of New Triphenylamine-Sensitized Solar Cells: a Theoretical Approach
Environ. Sci. Technol. (IF=4.825), **44** (2010) 5666–5671 [doi](#).
143. D. Jacquemin*, E. A. Perpète, F. Maurel and A. Perrier
TD-DFT Simulations of the Electronic Properties of Star-Shaped Photochromes
Phys. Chem. Chem. Phys. (IF=3.453), **12** (2010) 7994–8000 [doi](#).
144. C. A. Guido, B. Mennucci, D. Jacquemin and C. Adamo*
Planar vs. Twisted Intramolecular Charge Transfer Mechanism in Nile Red: New Hints from Theory
Phys. Chem. Chem. Phys. (IF=3.453), **12** (2010) 8016–8023 [doi](#).

145. D. Jacquemin*, C. Peltier and I. Ciofini*
On the Absorption Spectra of Recently Synthesized Carbonyl Dyes: TD-DFT Insights
J. Phys. Chem. A (IF=2.732), **114** (2010) 9579–9582 [doi](#).
146. D. Jacquemin*, E. A. Perpète, F. Maurel and A. Perrier
Hybrid Dithienylethene-Naphthopyran Multi-Addressable Photochromes: an Ab Initio Analysis
Phys. Chem. Chem. Phys. (IF=3.453), **12** (2010) 13144–13152 [doi](#).
147. A. Tabatchnik-Rebillon, C. Aubé, H. Bakkali, T. Delaunay, G. Thia Manh, V. Blot, C. Thobie-Gautier, E. Renault, A. Planchat, J. Y. Le Questel, B. Kauffmann, Y. Ferrand, I. Huc, K. Urgan, S. Condon, E. Léonel, M. Evain, J. Lebreton, D. Jacquemin, M. Pipelier and D. Dubreuil*
Electrochemical Synthesis and Characterisation of Alternated Tripyridyl-Dipyrrole Molecular Strands with Multi Nitrogen-Based Donor/Acceptor Binding Sites
Chem. Eur. J. (IF=5.476), **16** (2010) 11876–11889 [doi](#).
148. J. P. Cerón-Carrasco*, A. Requena, E. A. Perpète, C. Michaux and D. Jacquemin
Theoretical Study of the Tautomerism in One-Electron Oxidized Guanine-Cytosine Base Pair
J. Phys. Chem. B. (IF=3.603), **114** (2010) 13439–13445 [doi](#).
149. S. Chabbal*, D. Jacquemin, C. Adamo, H. Stoll and T. Leininger
Bond Length Alternation of Conjugated Oligomers: Another Step on the Fifth Rung of Perdew's Ladder of Functional
J. Chem. Phys. (IF=2.920), **133** (2010) 151104 (4 p.) [doi](#).
- Top 25 Hottest Articles**
150. J. Preat*, D. Jacquemin, C. Michaux and E. A. Perpète
Improvement of the Efficiency of Thiophene-Bridged Compounds for Dye-Sensitized Solar Cells
Chem. Phys. (IF=2.017), **376** (2010) 56–68 [doi](#).
- Most Read Articles**
151. C. A. Guido*, D. Jacquemin, C. Adamo and B. Mennucci
On the TD-DFT Accuracy in Determining Single and Double Bonds in Excited-State Structures of Organic Molecules
J. Phys. Chem. A (IF=2.732), **114** (2010) 13402–13410 [doi](#).
- Top 25 Hottest Articles**
152. D. Jacquemin*, E. A. Perpète, F. Maurel and A. Perrier*
Photochromic Properties of a Dithienylethene-Indolinoazolidine Switch: a Theoretical Investigation
Comput. Theor. Chem. (IF=1.437), **963** (2011) 63–70 [doi](#).
153. E. Dumont*, A. D. Laurent, X. Assfeld and D. Jacquemin
Performances of Recently-Proposed Functionals for Describing Disulfide Radical Anions and Similar Systems
Chem. Phys. Lett. (IF=2.337), **501** (2011) 245–251 [doi](#).
154. A. Perrier, F. Maurel, I. Ciofini and D. Jacquemin*
A Theoretical Spectroscopy Investigation of Bifunctional Platinum-Bridged Diarylethenes
Chem. Phys. Lett. (IF=2.337), **502** (2011) 77–81 [doi](#).
155. F. Maurel, A. Perrier and D. Jacquemin*
An ab initio Simulation of a Dithienylethene/Phenoxynaphthacenequinone Photochromic Hybrid
J. PhotoChem. PhotoBiol. A: Chem. (IF=2.421), **218** (2011) 33–40 [doi](#).
- Most Cited Articles**
HOT PAPERS
156. D. Jacquemin*, E. A. Perpète, I. Ciofini and C. Adamo*
Assessment of the ω B97 Family for Excited-state Calculations
Theor. Chem. Acc. (IF=2.162), **128** (2011) 127–136 [doi](#).
157. G. Revilla-Lopez, A. D. Laurent, E. A. Perpète, D. Jacquemin*, J. Torres, X. Assfeld* and C. Alemán*
Key Building Block of Photoresponsive Biomimetic Systems
J. Phys. Chem. B (IF=3.696), **115** (2011) 1232–1242 [doi](#).
- HIGHLY CITED**
158. D. Jacquemin* and C. Adamo*
Bond Length Alternation of Conjugated Oligomers: Wave Function and DFT Benchmarks
J. Chem. Theory Comput. (IF=5.215), **7** (2011) 369–376 [doi](#).



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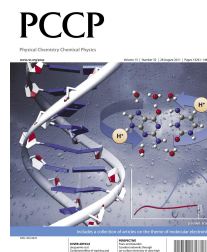
159. D. Jacquemin*
New Cyanine Dyes or Not ? Theoretical Insights for Model Chains
J. Phys. Chem. A (IF=2.946), **115** (2011) 2442–2445 [doi](#).
160. D. Jacquemin*, E. A. Perpète, C. Michaux and G. Frison*
Comparison of Microhydration Methods: Protonated Glycine as a Working Example
J. Phys. Chem. B. (IF=3.696), **115** (2011) 3604–3613 [doi](#).
161. Y. Pellegrin, L. Le Pleux, E. Blart, A. Renaud, B. Chavillon, N. Szuwarski, M. Boujtita, L. Cario, S. Jobic, D. Jacquemin* and F. Odobel*
Ruthenium Polypyridine Complexes as Sensitizers in NiO Based p-type Dye-Sensitized Solar Cells: Effects of the Anchoring Groups
J. PhotoChem. PhotoBiol. A: Chem. (IF=2.421), **219** (2011) 235–242 [doi](#).
162. A. Perrier*, F. Maurel and D. Jacquemin*
Interplay Between Electronic and Steric Effects in Multi-Photochromic Diarylethenes
J. Phys. Chem. C (IF=4.805), **115** (2011) 9193–9203 [doi](#).
163. A. Perrier, F. Maurel and D. Jacquemin*
Nature of the Excited-States in Large Photochromic Dimers: a TD-DFT Examination
Chem. Phys. Lett. (IF=2.337), **509** (2011) 129–133 [doi](#).
164. A. I. Gilson, G. van der Rest, J. Chamot-Rooke, W. Kurlancheek, M. Head-Gordon, D. Jacquemin and G. Frison*
Ground Electronic State of Peptide Cation Radicals: a Delocalized Unpaired Electron ?
J. Phys. Chem. Lett. (IF=6.213), **2** (2011) 1426–1431 [doi](#).
165. D. Jacquemin*, E. Bremond, A. Planchat, I. Ciofini and C. Adamo*
TD-DFT Vibronic Couplings in Anthraquinones: from Basis Set and Functional Benchmarks to Applications for Industrial Dyes
J. Chem. Theory Comput. (IF=5.215), **7** (2011) 1882–1892 [doi](#).
166. A. Perrier*, F. Maurel and D. Jacquemin*
Diarylethene-Dihydroazulene Multimode Photochrome: a Theoretical Spectroscopy Investigation
Phys. Chem. Chem. Phys. (IF=3.573), **13** (2011) 13791–13799 [doi](#).
167. J. P. Cerón-Carrasco*, J. Zúñiga, A. Requena, E. A. Perpète, C. Michaux and D. Jacquemin*
Combined Effect of Stacking and Solvation on the Spontaneous Mutation in DNA
Phys. Chem. Chem. Phys. (IF=3.573), **13** (2011) 14584–14589 [doi](#).
168. D. Jacquemin*, B. Mennucci* and C. Adamo*
Excited-State Calculations with TD-DFT: from Benchmarks to Simulations in Complex Environments
Phys. Chem. Chem. Phys. (IF=3.573), Perspective Article, **13** (2011) 16987–16998 [doi](#).

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169. J. P. Cerón-Carrasco* and D. Jacquemin*
Influence of Mg^{2+} on the Guanine-Cytosine Tautomeric Equilibrium: Simulations of the Induced Intermolecular Proton Transfer
ChemPhysChem (IF=3.412), **12** (2011) 2615–2623 [doi](#).
170. D. Jacquemin*, J. Preat, E. A. Perpète, D. P. Vercauteren, J. M. André, I. Ciofini and C. Adamo*
Absorption Spectra of Azobenzenes Simulated with Time-Dependent Density Functional Theory
Int. J. Quantum Chem. (IF=1.357), **111** (2011) 4224–4240 [doi](#).
171. J. Y. Le Questel*, J. Graton, J. P. Cerón-Carrasco, D. Jacquemin, A. Planchat and S. Thany*
New Insights on the Molecular Features, Electrophysiological Properties of Imidacloprid, Acetamiprid and Dinotefuran Neonicotinoid Insecticides
Bioorg. Med. Chem. (IF=2.921), **19** (2011) 7623–7634 [doi](#).
172. A. Tilborg, D. Jacquemin, B. Norberg, E. A. Perpète, C. Michaux and J. Wouters*
Structural Study of PIRACETAM Polymorphs and Cocrystals: Crystallography Redetermination and Quantum Mechanics Calculations
Acta Cryst. B (IF=2.286), **67** (2011) 499–507 [doi](#).



173. M. Cipolloni, A. Heynderickx, F. Maurel, A. Perrier, D. Jacquemin*, O. Siri, F. Ortica and G. Favaro*
A Multiswitchable Acidichromic and Photochromic bisDiarylethene. An Experimental and Theoretical Study
J. Phys. Chem. C (IF=4.805), **115** (2011) 23096–23106 [doi](#).
- Top 25**
Hottest Articles
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174. J. Warnan, L. Favereau, Y. Pellegrin, E. Blart, D. Jacquemin* and F. Odobel*
A Compact Diketopyrrolopyrrole Dye as Efficient Sensitizer in Titanium Dioxide Dye-Sensitized Solar Cells
J. PhotoChem. PhotoBiol. A: Chem. (IF=2.421), **226** (2011) 9–15 [doi](#).
175. J. P. Cerón-Carrasco, A. Ripoche, F. Odobel and D. Jacquemin*
Excited-State Nature in Benzodifuranone Dyes: Insights from ab initio Simulations
Dyes Pigm. (IF=3.532), **92** (2012) 1144–1152 [doi](#).
176. B. Le Guennic*, O. Maury and D. Jacquemin*
Aza-Boron-Dipyrromethene Dyes: TD-DFT Benchmarks, Spectral Analysis and Design of Original Near-IR Structures
Phys. Chem. Chem. Phys. (IF=3.829), **14** (2012) 157–164 [doi](#).
177. E. Cauët and D. Jacquemin*
A Theoretical Spectroscopy Investigation of Oxosumanenes
Chem. Phys. Lett. (IF=2.145), **519–520** (2012) 49–53 [doi](#).
- Editor's Choice**
178. J. Graton, J. Y. Le Questel, B. Legouin, P. Uriac, P. Van de Weghe and D. Jacquemin*
A DFT-D Evaluation of the Complexation of a Molecular Tweezer with Small Aromatic Molecules
Chem. Phys. Lett. (IF=2.145), **522** (2012) 11–16 [doi](#).
179. F. Maurel, A. Perrier and D. Jacquemin*
Ab Initio Modelling of Optical Spectra in pH-Sensitive Diarylethenes
Int. J. Quantum Chem. (IF=1.306), **112** (2012) 1122–1133 [doi](#).
180. D. Jacquemin*, E. Bremond, I. Ciofini and C. Adamo*
Impact of Vibronic Couplings on Perceived Colors: Two Anthraquinones as Working Example
J. Phys. Chem. Lett. (IF=6.585), **3** (2012) 468–471 [doi](#).
181. J. Hunault, M. Diswall, J. C. Frison, V. Blot, J. Rocher, S. Marionneau-Lambot, T. Oullier, J. Y. Douillard, S. Guillarme, C. Saluzzo, G. Dujardin, D. Jacquemin, J. Graton, J. Y. Le Questel, M. Evain, J. Lebreton, D. Dubreuil, J. Le Pendu and M. Pipelier*
3-Fluoro- and 3,3-Difluoro-3,4-dideoxy-KRN7000 Analogues as New Potent Immunostimulator Agents: Total Synthesis and Biological Evaluation in Human iNKT Cells and Mice
J. Med. Chem. (IF=5.614), **55** (2012) 1227–1241 [doi](#).
182. J. P. Cerón-Carrasco*, A. Requena and D. Jacquemin*
Impact of DFT Functionals on the Predicted Magnesium-DNA Interaction: an ONIOM Study
Theor. Chem. Acc. (IF=2.233), **131** (2012) 1188 (9 p.) [doi](#).
183. D. Jacquemin*
Spectroscopic Properties of Mono- and Bis-Azopyrroles
Int. J. Quantum Chem. (IF=1.306), **112** (2012) 2043–2050 [doi](#).
184. D. Jacquemin* and C. Adamo*
Basis Set and Functional Effects on Excited-State Properties: Three Bicyclic Chromogens as Working Examples
Int. J. Quantum Chem. (IF=1.306), **112** (2012) 2135–2141 [doi](#).
185. C. Dupont, E. Dumont* and D. Jacquemin*
Superior Performance of Range-Separated Hybrid Functionals for Describing $\sigma^ \leftarrow \sigma$ UV-Vis Signatures of Three-Electron Two-Center Anions*
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- Most Read Articles**
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On the Photochromic Properties of Dithienylethenes Grafted on Gold Clusters
Comput. Theor. Chem. (IF=1.371), **990** (2012) 167–176 [doi](#).

190. I. Ciofini, T. Le Bahers, C. Adamo, F. Odobel and D. Jacquemin*
Trough-Space Charge-Transfer in Rod-Like Molecules: Lessons from Theory
J. Phys. Chem. C (IF=4.814), **116** (2012) 11946–11955 [doi](#); errata: **116** (2012) 14736–14736 [doi](#).

191. D. E. López-Pérez, G. Revilla-López, D. Jacquemin, D. Zanuy, B. Palys, S. Sek* and C. Alemán*
Intermolecular Interactions in Electron Transfer through Stretched Helical Peptides
Phys. Chem. Chem. Phys. (IF=3.829), **14** (2012) 10332–10344 [doi](#).

192. D. Bousquet, C. Peltier, C. Masselin, D. Jacquemin, C. Adamo and I. Ciofini*
A DFT Study of Magnetic Interactions in Photoswitchable Systems: Diarylethene Derivatives
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Diketopyrrolopyrrole-Porphyrin Conjugates as Broadly Absorbing Sensitizers for Dye-Sensitized Solar Cells
ChemSusChem (IF=7.475), **5** (2012) 1568–1577 [doi](#).

195. P. O. Hubin, D. Jacquemin, L. Leherter, J. M. André, A. C. T. van Duin and D. P. Vercauteren*
Ab Initio Quantum Mechanical and ReaxFF-based Study of the Intramolecular Iminium-Enamine Conversion in a Proline-Catalyzed Reaction
Theor. Chem. Acc. (IF=2.233), **131** (2012) 1261 (11p) [doi](#).

196. A. Perrier, F. Maurel and D. Jacquemin*
Single Molecule MultiPhotochromism with Diarylethenes
Acc. Chem. Res. (IF=20.833), **45** (2012) 1173–1182 [doi](#).

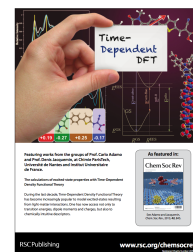
197. J. P. Cerón-Carrasco, D. Jacquemin* and E. Cauët
Cisplatin Cytotoxicity: a Theoretical Study of Induced Mutations
Phys. Chem. Chem. Phys. (IF=3.829), **14** (2012) 12457–12464 [doi](#).

198. S. Chibani, B. Le Guennic*, A. Charaf-Eddin, O. Maury, C. Andraud and D. Jacquemin*
On the Computation of Adiabatic Energies in Aza-Boron-Dipyrromethene Dyes
J. Chem. Theory Comput. (IF=5.389), **8** (2012) 3303–3313 [doi](#).

199. H. Nitadori, L. Ordronneau, J. Boixel, D. Jacquemin*, A. Boucekine, A. Singh, M. Akita, I. Ledoux, V. Guerchais and H. Le Bozec*
Photoswitching of the Second-order Nonlinearity of a Tetrahedral Octupolar Multi DTE-based Copolymer(I) Complex
Chem. Comm. (IF=6.378), **48** (2012) 10395–10397 [doi](#).

200. J. Graton*, B. Legouin, F. Besseau, P. Uriac, J. Y. Le Questel, P. van de Weghe and D. Jacquemin*
Molecular Tweezers in Host-Guest Complexes: A Computational Study through a DFT-D Approach
J. Phys. Chem. C (IF=4.814), **116** (2012) 23067–23074 [doi](#).

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 Inorg. Chem. (IF=4.593), **51** (2012) 11500–11512 [doi](#).
202. J. P. Cerón-Carrasco and D. Jacquemin*
Interplay Between Hydroxyl Radical Attack and H-bond Stability in Guanine-Cytosine
 RSC Adv. (IF=2.562), **2** (2012) 11867–11875 [doi](#).
203. F. B. Anne, N. Galland and D. Jacquemin*
Computing Redox Potentials for Dyes Used in p-type Dye-Sensitized Solar Cells
 Int. J. Quantum Chem. (IF=1.306), **112** (2012) 3763–3768 [doi](#).
204. J. P. Cerón-Carrasco, M. Fanuel, A. Charaf-Eddin and D. Jacquemin*
Interplay Between Solvent Models and Predicted Optical Spectra: a TD-DFT Study of 7-OH-Coumarin
 Chem. Phys. Lett. (IF=1.991), **556** (2013) 122–126 [doi](#).
205. U. Bussy, I. Tea, V. Ferchaud-Roucher, M. Krempf, V. Silvestre, N. Galland, D. Jacquemin, M. Andresen-Bergström, U. Jurva and M. Boujtita*
Mass Voltammetry Technique in the Presence of Isotopic ¹⁸O Labelled Water For the Prediction of Oxidative Metabolism
 Anal. Chim. Acta (IF=4.517), **762** (2013) 39–46 [doi](#).
206. C. Adamo and D. Jacquemin*
The Calculations of Excited-State Properties with Time-Dependent Density Functional Theory
HIGHLY CITED Chem. Soc. Rev. (IF=30.425), *invited tutorial review*, **42** (2013) 845–856 [doi](#).
207. J. P. Cerón-Carrasco* and D. Jacquemin
Electric-Field Induced Mutation on DNA: a Theoretical Investigation of the GC Base Pair
 Phys. Chem. Chem. Phys. (IF=4.198), **15** (2013) 4548–4553 [doi](#).
 Part of the *great articles recently published in the fields of biophysics and biophysical chemistry*.
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209. S. Chibani, B. Le Guennic*, A. Charaf-Eddin, A. D. Laurent and D. Jacquemin*
Revisiting the Optical Signatures of BODIPY with Ab Initio Tools
 Chem. Sci. (IF=8.601), **4** (2013) 1950–1963 [doi](#).
210. S. Aloïse*, M. Silwa, G. Buntinx, S. Delbaere, A. Perrier, F. Maurel, D. Jacquemin and M. Takeshita
Do Inverse Dithienylethene Behave as Normal One ? A Joint Spectroscopic and Theoretical Investigation
 Phys. Chem. Chem. Phys. (IF=4.198), **15** (2013) 6226–6234 [doi](#).
211. J. P. Cerón-Carrasco*, D. Jacquemin, J. Graton, S. Thany and J. Y. Le Questel*
New Insights on the Molecular Recognition of Imidacloprid with Aplysia Californica AChBP : a Computational Study
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Ruthenium Sensitizer Functionalized by Acetylacetone Anchoring Groups for Dye-Sensitized Solar Cells
 J. Phys. Chem. C (IF=4.835), **117** (2013) 8652–8660 [doi](#).



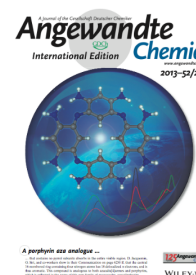
214. B. Le Guennic*, S. Chibani, A. Charaf-Eddin, J. Massue, R. Ziessel, G. Ulrich* and D. Jacquemin*
The NBO Pattern in Luminescent Chromophores: Unravelling Excited-State Features with TD-DFT
Phys. Chem. Chem. Phys. (IF=4.189), **15** (2013) 7534–7540 [doi](#).
215. L. Ordonneau, V. Aubert, V. Guerchais, A. Boucekkine, H. Le Bozec*, A. Singh, I. Ledoux, and D. Jacquemin*
The First Hexa-Dithienylethene Tris(Bipyridine)Metal complexes as Quadratic NLO Photoswitches: Combined Experimental and DFT Studies
Chem. Eur. J. (IF=5.696), **19** (2013) 5845–5849 [doi](#).
216. D. Bousquet, R. Fukuda, P. Maitrad, D. Jacquemin, I. Ciofini, C. Adamo* and M. Ehara*
Excited-State Geometries of Heteroaromatic Compounds: a Comparative TD-DFT and SAC-CI Study
J. Chem. Theory Comput. (IF=5.310), **9** (2013) 2368–2379 [doi](#).
217. J. Massin, A. Charaf-Eddin, F. Appaix, Y. Bretonnière, D. Jacquemin*, B. Van der Sanden*, C. Monnerneau* and C. Andraud
A Water Soluble Probe with Polarity-Induced near Infra-Red Fluorescence and its use in Two-Photon Cerebral Vasculature Imaging
Chem. Sci. (IF=8.610), **4** (2013) 2833–2843 [doi](#).
218. Z. Chen, M. Giorgi, D. Jacquemin*, M. Elhabiri and O. Siri*
Azacalixphyrin: the Hidden Porphyrin Cousin Brought to Light
Angew. Chem. Int. Ed. (IF=11.336), **52** (2013) 6250–6254 [doi](#).
Selected in Synfacts **9** (2013) 0838 [doi](#).
219. A. Charaf-Eddin, A. Planchat, B. Mennucci*, C. Adamo* and D. Jacquemin*
Choosing a Functional for Computing Absorption and Fluorescence Band Shapes with TD-DFT
J. Chem. Theory Comput. (IF=5.310), **9** (2013) 2749–2760 [doi](#).
220. L. Favereau, J. Warnan, F. B. Anne, Y. Pellegrin, E. Blart, D. Jacquemin* and F. Odobel*
Diketopyrrolopyrrole-Zinc Porphyrin, a Tuned Panchromatic Association for Dye-Sensitized Solar Cells
J. Mater. Chem. A (IF=7.443), **1** (2013) 7572–7575 [doi](#).
221. A. Perrier*, S. Aloïse, M. Olivucci* and D. Jacquemin*
Inverse versus Normal Dithienylethenes: A Theoretical investigation of the Photocyclization Reaction
J. Phys. Chem. Lett. (IF=6.687), **4** (2013) 2190–2196 [doi](#).
222. U. Bussy, M. Delaforge, C. El-Bekkali, V. Ferchaud-Roucher, M. Krempf, I. Tea, N. Galland, D. Jacquemin and M. Boujtita*
Acebutolol and Alprenolol Metabolism Predictions: Comparative Study of Electrochemical and Cytochrome P450-Catalyzed Reactions Using Liquid Chromatography Coupled to High-Resolution Mass Spectrometry
Anal. Bioanal. Chem. (IF=3.578), **405** (2013) 6077–6085 [doi](#).
223. Y. Houari, D. Jacquemin and A. D. Laurent*
Methodological Keys for Accurate pK_a^ Simulations*
Phys. Chem. Chem. Phys. (IF=4.189), **15** (2013) 11875–11882 [doi](#).
224. S. Chibani, A. Charaf-Eddin, B. Le Guennic* and D. Jacquemin*
Boranil and Related NBO Dyes: Insights From Theory
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225. A. Faucon, R. Lenk, J. Hémez, E. Gautron, D. Jacquemin, J.Y. Le Questel, J. Graton, A. Brosseau and E. Ishow*
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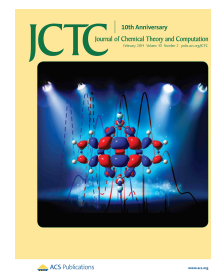
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Electric Field Induced DNA Damage: an Open Door for Selective Mutations
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Optical Signatures of Boron Adducts of Oxasmaragdyrin: Insights from Theory
Mol. Phys. (IF=1.642), **111** (2013) 1303–1307 [doi](#).
229. F. B. Anne, F. D. Purpan and D. Jacquemin*
Charge-Transfer in QuasiLinear Push-Pull Polyene Chains
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230. K. Yuan, J. Boixel, H. Le Bozec, A. Boucekkine, H. Doucet*, V. Guerchais* and D. Jacquemin*
Perfluorocyclohexene Bridges in Inverse Diarylethenes: Synthesis through Pd-Catalysed C-H bond Activation, Experimental and Theoretical Studies on Their Photoreactivity
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Probing the Performances of HISS Functionals for the Description of Excited States of Molecular Systems
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Is the Tamm-Dancoff Approximation Reliable for the Calculation of Absorption and Fluorescence Band Shapes?
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Design of Hybrid Conjugates Based on Chemical Similarity
RSC Adv. (IF=3.708), **3** (2013) 21069–21083 [doi](#).
237. Y. Houari, A. D. Laurent and D. Jacquemin*
Spectral Signatures of Perylene Diimide Derivatives: Insights from Theory
J. Phys. Chem. C (IF=4.835), **117** (2013) 21682–21691 [doi](#).
238. O. Selaimia-Ferdjani, A. Kar, S. P. Chavan, M. Horeau, G. Viault, J. Pouessel, X. Guillory, V. Blot, A. Tessier, C. Bidjou-Haiour, A. Planchat, D. Jacquemin, D. Dubreuil and M. Pipelier*
Stereoselective Synthesis of a Bicyclic Norsesquiterpene Backbone. A Possible Route to Nardosinane Derivatives
Eur. J. Org. Chem. (IF=3.154), (2013) 7083–7094 [doi](#).
239. K. Beydoun, M. Zaarour, J. A. Gareth Williams, T. Roisnel, V. Dorcet, A. Planchat, A. Boucekkine, D. Jacquemin*, H. Doucet* and V. Guerchais*
Palladium-Catalysed Direct Arylation of Luminescent Bis-Cyclometallated Iridium(III) Complex Incorporating $\hat{\text{C}}\text{N}$ - or $\text{O}\hat{\text{O}}$ -Coordinating Thiophene-Based Ligands: an Efficient Method for Color tuning
Inorg. Chem. (IF=4.794), **52** (2013) 12416–12428 [doi](#).



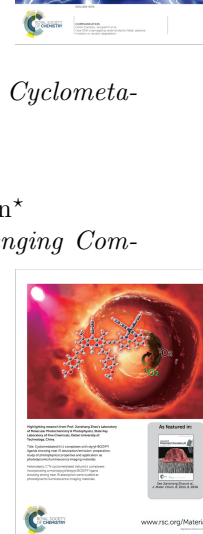
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Pretreatment of the Cockroach Cercal Afferent/Giant Interneuron Synapses with Nicotinoids and Neonicotinoids Differently Affects Acetylcholine and Nicotine-Induced Ganglionic Depolarizations
Invertebr. Neurosci. (IF=1.192), **13** (2013) 91–97 [doi](#).
241. S. Aiken, C. D. Gabbutt, L. J. Gillie, J. D. Heywood, D. Jacquemin, C. R. Rice and B. M. Heron*
The Remarkable Hyperchromicity of Ketohydrazone Dyes and Pigment Lakes Derived from 4-Morpholino-2-Naphthol
Eur. J. Org. Chem. (IF=3.154), (2013) 8097–8107 [doi](#).
242. J. P. Ceron-Carrasco*, D. Jacquemin and E. Dumont*
Impact of DNA Environment on the Intrastrand Cross-Link Lesions: Hydrogen Atom Release as the Last Step of Formation of G[8-5m]/T
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243. Y. Houari, A. Charaf-Eddin, A. D. Laurent, J. Massue, R. Ziessel, G. Ulrich and D. Jacquemin*
Modeling Optical Signatures and Excited-State Reactivities of Substituted HydroxyphenylBenzOxazoles (HBO) ESIPT Dyes
Phys. Chem. Chem. Phys. (IF=4.493), **16** (2014) 1319–1321 [doi](#).
244. A. Charaf-Eddin, B. Le Guennic, and D. Jacquemin*
Optical Signatures of Borico Dyes: a TD-DFT Analysis
Theor. Chem. Acc. (IF=2.233), **133** (2014) 1456 (9p) [doi](#).
245. S. Chibani, A. Charaf-Eddin, B. Mennucci*, B. Le Guennic* and D. Jacquemin*
Optical Signatures of OBO Fluorophores: a Theoretical Analysis
J. Chem. Theory Comput. (IF=5.498), **10** (2014) 805–815 [doi](#).
246. K. J. Chen, A. D. Laurent and D. Jacquemin*
Strategies for Designing Diarylethenes as Efficient Nonlinear Optical Switches
J. Phys. Chem. C (IF=4.772), **118** (2014) 4334–4345 [doi](#).
247. J. Warnan, Y. Pellegrin, E. Blart, L. Zhang, A. Brown, L. Hammarström*, D. Jacquemin* and F. Odobel*
Acetylacetone Anchoring Group for NiO-Based Dye-Sensitized Solar Cell
Dyes Pigm. (IF=3.966), **105** (2014) 174–179 [doi](#).
248. X. Cui, A. Charaf-Eddin, J. Wang, B. Le Guennic, J. Zhao* and D. Jacquemin*
Perylene-Derived Triplet Acceptors with Optimized Excited State Energy Levels for Triplet-triplet Annihilation Upconversion
J. Org. Chem. (IF=4.721), **79** (2014) 2038–2048 [doi](#).
249. P. Boulanger, D. Jacquemin*, I. Duchemin and X. Blase*
Fast and Accurate Electronic Excitations in Cyanines with the Many-Body Bethe-Salpeter Approach
J. Chem. Theory Comput. (IF=5.498), **10** (2014) 1212–1218 [doi](#).
250. P. O. Hubin*, D. Jacquemin, L. Leherter and D. P. Vercauteren
Quantum Mechanical Investigations on the Role of Neutral and Negatively Charged Enamine Intermediates in Organocatalyzed Reactions
Chem. Phys. (IF=1.652), **434** (2014) 30–36 [doi](#).
251. A. D. Laurent*, Y. Houari, P. H. P. R. Carvalho, B. A. D. Neto and D. Jacquemin*
ESIPT or not ESIPT ? Revisiting Recent Results on 2,1,3-Benzothiadiazole under the TD-DFT Light
RSC Adv. (IF=3.840), **4** (2014) 14189–14192 [doi](#).
252. N. Oger, F. Le Callonnec, D. Jacquemin*, E. Fouquet, E. Le Grogneec and F.X. Felpin*
Heck-type Arylation of Olefins Through a Double Catalytic Activation of Anilines: Improved Procedures and Rationalization
Adv. Synth. Catal. (IF=5.663), **356** (2014) 1065–1071 [doi](#).



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253. J. P. Ceron-Carrasco, H. M. Roy, J. Cerezo, D. Jacquemin and A. D. Laurent*
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Chem. Phys. Lett. (IF=1.897), **599** (2014) 73–79 [doi](#).
254. D. Jacquemin*, B. Moore II, A. Planchat, C. Adamo and J. Autschbach*
Performance of an Optimally-Tuned Range-Separated Hybrid Functional for 0-0 Electronic Excitation Energies
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255. J. P. Ceron-Carrasco*, J. Cerezo and D. Jacquemin*
How DNA is Damaged by External Electric Fields: Selective Mutation vs. Random Degradation
Phys. Chem. Chem. Phys. (IF=4.493), **16** (2014) 8243–8246 [doi](#).
256. J. Boixel, V. Guerchais*, H. Le Bozec, D. Jacquemin*, A. Amar*, A. Boucekkine*, A. Colombo, C. Dragonetti, D. Marinotto, D. Roberto*, S. Righetto and R. De Angelis
Second-Order NLO switches from Molecules to Polymer Films Based on Photochromic Cyclometalated platinum(II) Complexes
J. Am. Chem. Soc. (IF=12.113), **136** (2014) 5367–5375 [doi](#).
257. C. Katan*, P. Savel, B. M. Wong, T. Roisnel, V. Dorcet, J. L. Fillaut and D. Jacquemin*
Absorption and Fluorescence Signatures of 1,2,3-Triazole Based Regioisomers : Challenging Compounds for TD-DFT
Phys. Chem. Chem. Phys. (IF=4.493), **16** (2014) 9064–9073 [doi](#).
258. P. Majumdar, X. Yuan, S. Li, B. Le Guennic, J. Ma, C. Zhang, D. Jacquemin and J. Zhao*
Cyclometalated Ir(III) Complex with Styryl-Bodipy Ligands Showing Near IR Absorption/Emission: Preparation, Study of Photophysical Properties and Application as Photodynamic/Luminescence Imaging Materials
J. Mater. Chem. B (IF=4.726), **2** (2014) 2838–2854 [doi](#).
259. A. Honraedt, M. A. Raux, E. Le Grogne, D. Jacquemin and F. X. Felpin*
Copper-Catalyzed Free-Radical C-H Arylation of Pyrroles
Chem. Comm. (IF=6.834), **50** (2014) 5236–5238 [doi](#).
260. J. P. Ceron-Carrasco, D. Jacquemin, C. Laurence*, A. Planchat, C. Reichardt and K. Sraïdi²
Determination of a Solvent Hydrogen-bond Acidity Scale by Means of the Solvatochromism of Pyridinium-N-Phenolate Betaine Dye 30 and PCM-TD-DFT Calculations
J. Phys. Chem. B (IF=3.302), **118** (2014) 4605–4614 [doi](#).
261. S. Chibani, A. D. Laurent, A. Blondel, B. Mennucci* and D. Jacquemin*
Excited-State Geometries of Solvated Molecules: Going Beyond the Linear-Response Polarizable Continuum Model
J. Chem. Theory Comput. (IF=5.498), **10** (2014) 1848–1851 [doi](#).
262. J. P. Ceron-Carrasco, D. Jacquemin, C. Laurence*, A. Planchat, C. Reichardt and K. Sraïdi³
Solvent Polarity Scales: Determination of New $E_T(30)$ Values for 84 Organic Solvents
J. Phys. Org. Chem. (IF=1.380), **27** (2014) 512–518 [doi](#).
263. A. D'Aléo*, H. Vasile, G. Michel, B. Le Guennic*, D. Jacquemin and F. Fages
NIR Emission in Borondifluoride Complexes of 2'-Hydroxychalcone Derivatives Containing an Acetonaphthone Ring
J. Phys. Chem. C (IF=4.772), **118** (2014) 11906–11918 [doi](#).
264. S. Pascal, A. Haeefe, C. Monnereau, A. Charaf-Eddin, D. Jacquemin, B. Le Guennic*, C. Andraud* and O. Maury*
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J. Phys. Chem. Lett. (IF=7.458), **5** (2014) 2254–2258 [doi](#).
266. S. Aiken, K. Booth, C. D. Gabbutt, M. Heron*, C. R. Rice, A. Charaf-Eddin and D. Jacquemin
The First Structural and Spectroscopic Characterisation of a Ring-Opened Form of a 2H-Naphtho[1,2-b]pyran; a Novel Photomerocyanine
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Synthesis, Photovoltaic Performances and ab initio Modeling of Push-Pull Diacetylide Platinum Complexes in TiO₂ based Dye-Sensitized Solar Cells
Dalton Tans. (IF=4.197), *invited paper*, **43** (2014) 11233–11242 [doi](#).
269. A. Steffen*, K. Costuas*, A. Boucekkine, M. H. Thibault, A. Beeby, A. S. Batsanov, A. Charaf-Eddin, D. Jacquemin, J.F. Halet and T. B. Marder*
Fluorescence in Rhoda- and Iridacyclopentadienes Neglecting the Heavy Atom's Spin-Orbit Coupling: The Ligand Wins
Inorg. Chem. (IF=4.762), **53** (2014) 7055–7069 [doi](#).
270. J. Massue*, K. Benelhadj, S. Chibani, B. Le Guennic, D. Jacquemin*, P. Retailleau, G. Ulrich* and R. Ziessel*
Fluorescent 2-(2'-Hydroxybenzofurane)benzoxazole (HBBO) Borate Complexes: Synthesis, Optical Properties and Theoretical Simulations
Tetrahedron Lett. (IF=2.379), **55** (2014) 4136–4140 [doi](#).
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The Solvatomagnetic Comparison Method: a Proper Quantification of Solvent Hydrogen-Bond Basicity
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272. S. Chibani, D. Jacquemin* and A. D. Laurent
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Unveiling Solvents Effect on Excited-State Polarizabilities with the Corrected Linear-Response Model
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275. K. Yuan, J. Boixel, A. Chantzis, D. Jacquemin*, V. Guerschais* and H. Doucet*
Benzothiophene or Benzofuran Bridges in DiArylEthenes: Two Steps Synthesis through Sequential Pd-Catalysed C-H bond Activations and Joint Theoretical-Experimental Studies on Their Photoreactivity
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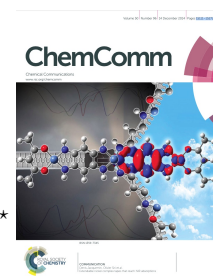
277. V. Riffet, D. Jacquemin, E. Cauët and G. Frison*
Benchmarking DFT and TD-DFT Functionals for the Ground and Excited States of Hydrogen-Rich Peptide Radicals
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Aggregation Effect on the Luminescence Properties of Phenyl Bipyridine Pt(II) Acetylide Complexes. A Theoretical Prediction with Experimental Evidence.
J. Phys. Chem. A (IF=2.693), **118** (2014) 6278–6286 [doi](#).
279. D. Jacquemin, J. Zuniga, A. Requena and J. P. Ceron-Carrasco*
Assessing the Importance of Proton Transfer Reactions in DNA
Acc. Chem. Res. (IF=22.323), **47** (2014) 2467–2474 [doi](#).
280. A. Chantzis, J. Cerezo, A. Perrier, F. Santoro* and D. Jacquemin*
Optical Properties of Diarylethenes with TD-DFT: 0-0 Energies, Fluorescence, Stokes Shifts and Vibronic Shapes
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281. D. Bousquet, R. Fukuda, D. Jacquemin, I. Ciofini, C. Adamo* and M. Ehara*
Benchmark Study on the Triplet Excited-State Geometries and Phosphorescence Energies of Heterocyclic Compounds: Comparison between TD-PBE0 and SAC-CI
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282. K. Benelhadj, W. Muzuzu, J. Massue*, P. Retailleau, A. Charaf-Eddin, A. D. Laurent, D. Jacquemin*, G. Ulrich* and R. Ziessel*
White Solid-State Emitters by Tuning the Excited State Intramolecular Proton Transfer (ESIPT) Fluorescence Emission in 2-(2'-Hydroxybenzofuran)benzoxazole (HBBO) Dyes
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283. G. Marchand*, A. D. Laurent, Z. Chen, O. Siri and D. Jacquemin*
The Exceptional Stability of Azacalixpyrin and its Dianion
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Competitive Direct versus Indirect Photochromism Dynamics in Constrained Inverse Dithienylethene Molecules
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Analyzing Excited-State Processes and Optical Signatures of a Ratiometric Fluorine Anion Sensor: a Quantum Look
Sc. China Chem. (IF=1.695), **57** (2014) 1363–1368 [doi](#).
286. A. Charaf-Eddin, B. Le Guennic* and D. Jacquemin*
Excited-States of BODIPY-Cyanines: Ultimate TD-DFT Challenges ?
RSC Adv. (IF=3.840), **4** (2014) 49449–49456 [doi](#).
287. P. Boulanger, S. Chibani, B. Le Guennic, I. Duchemin X. Blase* and D. Jacquemin*
Combining the Bethe-Salpeter Formalism with Time-Dependent DFT Excited-State Forces to Describe Optical Signatures: NBO Fluoroborates as Working Examples
J. Chem. Theory Comput. (IF=5.498), **10** (2014) 4548–4556 [doi](#).
288. S. Chibani, A. D. Laurent*, B. Le Guennic* and D. Jacquemin*
Improving the Accuracy of Excited State Simulations of BODIPY and aza-BODIPY Dyes with a Joint SOS-CIS(D) and TD-DFT Approach
J. Chem. Theory Comput. (IF=5.498), **10** (2014) 4574–4582 [doi](#).
289. B. Moore II, A. Charaf-Eddin, A. Planchat, C. Adamo, J. Autschbach* and D. Jacquemin*
Electronic Band Shapes Calculated with Optimally-Tuned Range-Separated Hybrid Functionals
J. Chem. Theory Comput. (IF=5.498), **10** (2014) 4599–4608 [doi](#).

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Investigation of ESIPT in a Panel Chromophores Presenting N-H...N Intramolecular Hydrogen Bonds
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292. H. Audi, Z. Chen, A. Charaf-Eddin, A. D'aléo, G. Canard, D. Jacquemin* and O. Siri*
Extendable Nickel Complex Tapes
Chem. Comm. (IF=6.834), **50** (2014) 15140–15143 [doi](#).



293. K. Benelhadj, J. Massue*, P. Retailleau, S. Chibani, B. Le Guennic, D. Jacquemin*, G. Ulrich* and R. Ziessel*
Solution- and Solid-State Luminescent Borate Complexes Based on a Substituted Π -Conjugated 2-(2'-hydroxybenzofuran) Scaffold
Eur. J. Org. Chem. (IF=3.065), (2014) 7156–7164 [doi](#).

294. S. Chibani, S. Budzak, M. Medved, B. Mennucci* and D. Jacquemin*
Full cLR-PCM Calculations of the Solvatochromic Effects on Emission Energies
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295. S. Aloïse*, R. Yibin, H. Ismail, G. Buntinx, A. Perrier*, F. Maurel, D. Jacquemin* and M. Takeshita
The Photochemistry of Inverse Dithienylethene Switches Understood
Phys. Chem. Chem. Phys. (IF=4.493), **16** (2014) 26762–26768 [doi](#).

296. T. Jaunet-Lahary, A. Chantzis*, K. J. Chen, A. D. Laurent and D. Jacquemin*
Designing Efficient Azobenzene and Azothiophene Nonlinear Optical Photochromes
J. Phys. Chem. C (IF=4.772), **118** (2014) 28831–28841 [doi](#).

297. U. Bussy, U. Jurva, R. Boisseai, M. Andresen-Bergström, V. Silvestre, N. Galland, D. Jacquemin and M. Boujtita*
Unexpected Benzimidazol Ring Formation from Quinoneimide Species in the Presence of Ammonium Acetate as Supporting Electrolyte Used in the Coupling Electrochemistry with Mass Spectrometry
Rapid Commun. Mass Spectrom. (IF=2.226), **29** (2015) 456–460 [doi](#).

298. A. Maufroy, L. Favereau, F. B. Anne, Y. Pellegrin, E. Blart, M. Hissler, D. Jacquemin* and F. Odobel*
Synthesis and Properties of Push-Pull Porphyrins as Sensitizers for NiO Based Dye-Sensitized Solar Cells
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N-Confused Porphyrin Tautomers: Lessons from Density Functional Theory
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300. Y. Houari, S. Chibani, D. Jacquemin and A. D. Laurent*
A TD-DFT Assessment of the Excited State Intramolecular Proton Transfer in HydroxyphenylBenzimidazole (HBI) Dyes
J. Phys. Chem. B (IF=3.187), **119** (2015) 2180–2192 [doi](#).

301. C. Laurence*, J. Legros, A. Chantzis, A. Planchat and D. Jacquemin
A Database of Dispersion-Induction DI, Electrostatic ES, and Hydrogen Bonding α_1 and β_1 Solvent Parameters and Some Applications
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302. K. J. Chen, A. Charaf-Eddin, B. Selvam, F. Boucher, A. D. Laurent and D. Jacquemin*
Interplay Between TiO₂ Surface and Organic Photochromes: A DFT Study Of Adsorbed Azobenzenes and Diarylethenes
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Dissymmetric Molecular Tweezers in Host-Guest Complexes: Internal or External Complexation ?
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Excited-State Vibrations of Solvated Molecules: Going Beyond the Linear-Response Polarizable Continuum Model
J. Chem. Theory Comput. (IF=5.301), **11** (2015) 847–859 [doi](#).
305. J. P. Ceron-Carrasco*, A. Requena, J. Zuniga and D. Jacquemin
Mutagenic Effects Induced by the Attack of NO₂ Radical to the Guanine-Cytosine Base Pair
Front. Chem. (IF=N/A), **3** (2015) 13 (7p) [doi](#).
- chemistryworld**
306. J. P. Ceron-Carrasco* and D. Jacquemin
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Sequential Double Second-Order Nonlinear Optical Switch by an Acido-Triggered Photochromic Cyclometallated Platinum(II) Complex
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Computational insights into the photodeactivation dynamics of phosphors for OLEDs: a Perspective
Dalton Tans. (IF=4.177), *perspective*, **44** (2015) 8346–8355 [doi](#).
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Designing Efficient Photochromic Dithienylethene Dyads
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Choosing an Atomic Basis Set for TD-DFT, SOPPA, ADC(2), CIS(D), CC2 and EOM-CCSD Calculations of Low-Lying Excited-States of Organic Dyes
Theor. Chem. Acc. (IF=1.806), **134** (2015) 76 (11p) [doi](#).
313. S. Chibani, A. D. Laurent, B. Le Guennic* and D. Jacquemin*
Excited States of Ladder-Type π -conjugated Dyes with a Joint SOS-CIS(D) and PCM-TD-DFT Approach
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315. S. Ji,* J. Ge, D. Escudero, Z. Wang, J. Zhao,* and D. Jacquemin*
Molecular Structure-Intersystem Crossing Relationship of Heavy Atom-Free BODIPY Triplet Photosensitizers
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316. A. Felouat, A. D'Aléo, A. Charaf-Eddin, D. Jacquemin, B. Le Guennic*, E. Kim, K. J. Lee, J. H. Woo, J.C. Ribierre, J. W. Wu* and F. Fages*

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Tetrahedron (IF=2.645), **71** (2015) 7676–7680 [doi](#).

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324. D. Ameline, S. Diring, Y. Farre, Y. Pellegrin, G. Naponiello, E. Blart, B. Charrier, D. Dini, D. Jacquemin* and F. Odobel*

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RSC Adv. (IF=3.289), **5** (2015) 85530–85539 [doi](#).

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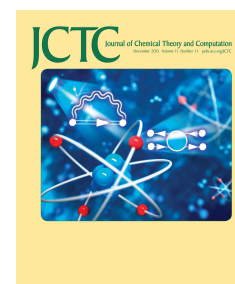
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333. E. Kim, A. Felouat, E. Zaborova, J. C. Ribierre, J. W. Wu, S. Senatore, C. Matthews, P. F. Lenne, C. Baffert, A. Karapetyan, M. Giorgi, D. Jacquemin, M. A. Ponce-Vargas, B. Le Guennic, F. Fages and A. D'Aleo*

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338. R. Beneteau, A. Boussonniere, J. C. Rouaud, J. Lebreton, J. Graton, D. Jacquemin, M. Sebban, H. Oulyadi, G. Hamdoun, A. N. Hancock, C. H. Schiesser and F. Denes*

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340. G. Marchand*, P. Giraudeau, Z. Chen, O. Siri* and D. Jacquemin*

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Phys. Chem. Chem. Phys. (IF=4.123), **18** (2016) 9608–9615 [doi](#).

341. K. Kamada*, T. Namikawa, S. Senatore, C. Matthews, P. F. Lenne, O. Maury, C. Andraud, M. A. Ponce Vargas, B. Le Guennic, D. Jacquemin, P. Agbo, D. D. An, S. S. Gauny, X. Liu, R. J. Abergel*, F. Fages and A. D'Aleo*

Borondifluoride Curcuminoid Fluorophores with Enhanced Two-Photon Excited Fluorescence Emission and Versatile Living-Cell Imaging Properties

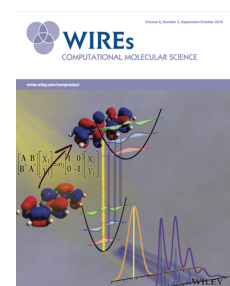
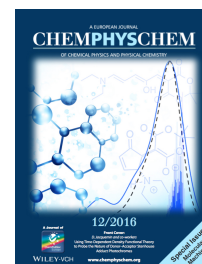
Chem. Eur. J. (IF=5.317), **22** (2016) 5219–5232 [doi](#).



342. S. Budzak, A. D. Laurent, C. Laurence, M. Medved and D. Jacquemin*
Solvatochromic Shifts in UV-Vis Absorption Spectra: The Challenging Case of 4-Nitropyridine N-Oxide
J. Chem. Theory Comput. (IF=5.245), **12** (2016) 1919–1929 [doi](#).
343. D. Jacquemin*, I. Duchemin and X. Blase*
Assessment of the Convergence of Partially Self-Consistent BSE/GW Calculations
Mol. Phys. (IF=1.870), **114** (2016) 957–967 [doi](#).
344. Y. Farre, L. Zhang, Y. Pellegrin, A. Planchat, E. Blart, M. Boujtita, L. Hammarstrom*, D. Jacquemin* and F. Odobel*
Second Generation of Diketopyrrolopyrrole Dyes for NiO Based Dye-Sensitized Solar Cells
J. Phys. Chem. C (IF=4.536), **120** (2016) 7923–7940 [doi](#).
345. P. Le Pogam, A.-C. Le Lamer, S. Bandi, B. Legouin, A. Bondon, J. Graton, D. Jacquemin, P. Uriac, I. Rouaud, S. Ferron, W. Obermayer, K. Suresh Babu and J. Boustie*
Minor Naphthazarinopyranones from Lichen Ophioparma Ventosa Apotheciae
J. Nat. Prod. (IF=3.281), **79** (2016) 1005–1011 [doi](#).
346. I. Duchemin*, D. Jacquemin and X. Blase
Combining the GW Formalism with the Polarizable Continuum Model : a State-Specific Non-Equilibrium Approach
J. Chem. Phys. (IF=2.965), **144** (2016) 164106 (13 p) [doi](#).
347. E. Hitti, B. Legouin, J. Graton, D. Jacquemin and P. Uriac*
¹H NMR and Computational Studies of the Conformations in Solution of one Host/Guest Complex Formed with an Usnic Acid Tweezer and 2,4,7-Trinitro-9-fluorenone (TNF)
Tetrahedron (IF=2.651), **72** (2016) 2890–2894 [doi](#).
348. C. Azarias and D. Jacquemin*
Elucidating the Nature of Carbazole-Porphyrinoids with First-Principle Approaches
J. Phys. Chem. A (IF=2.847), **120** (2016) 2824–2831 [doi](#).
349. S. Pascal, C. Besnard, F. Zinna, L. Di Bari, B. Le Guennic, D. Jacquemin and J. Lacour*
Zwitterionic [4]Helicene: a Water-Soluble and Reversible pH Triggered ECD/CPL Chiroptical Switch in the UV and Red Spectral Regions
Org. Biomol. Chem. (IF=3.564), **14** (2016) 4590–4594 [doi](#).
350. W. Yang, J. Zhao,* C. Sonn, D. Escudero, A. Karatay, H. G. Yaglioglu, B. Küçüköz, M. Hayvali,* C. Li,* and D. Jacquemin*
Efficient Intersystem Crossing in Heavy atom-Free Perylenebisimide Derivatives
J. Phys. Chem. C (IF=4.536), **120** (2016) 10162–10175 [doi](#).
351. C. Azarias, S. Budzak, A. D. Laurent, G. Ulrich and D. Jacquemin*
Tuning ESIPT Fluorophores into Dual Emitters
Chem. Sci. (IF=8.668), **7** (2016) 3763–3774 [doi](#).
352. A. Fihey* and D. Jacquemin*
How Metals Can Help Multiphotochromism: an Ab Initio Study
J. Phys. Chem. C (IF=4.536), **120** (2016) 11140–11150 [doi](#).
353. M. C. Chang, A. Chantzis, D. Jacquemin and E. Otten*
Boron Difluorides with Formazanate Ligands: Redox-Switchable Fluorescent Dyes with Large Stokes Shifts
Dalton Trans. (IF=4.029), **45** (2016) 9477–9484 [doi](#).
354. M. d'Halluin, J. Rull-Barrull, E. Le Grogne, D. Jacquemin and F.X. Felpin*
Writing and Erasing Hidden Optical Information on Covalently Modified Cellulose Paper
Chem. Comm. (IF=6.319), **52** (2016) 7672–7675 [doi](#).
355. A. Prlj, M. E. Sandoval-Salinas, D. Casanova, D. Jacquemin* and C. Corminboeuf*
Low Lying $\pi\pi^$ States of Heteroaromatic Molecules: A Challenge for Excited State Methods*
J. Chem. Theory Comput. (IF=5.245), **12** (2016) 2652–2660 [doi](#).

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356. A.D. Laurent, M. Medved' and D. Jacquemin*
Using TD-DFT to Probe the Nature of Donor-Acceptor Stenhouse Adduct Photochromes
 ChemPhysChem (IF=3.075), **17** (2016) 1846–1851 [doi](#).
357. B. Jedrzejewska, A. Zakrzewska, G. Mloston, S Budzak, K. Mroczynska, A. M. Grabarz, M. Kaczorowska, D. Jacquemin and B. Osmialowski*
Synthesis and Photophysical Properties of Novel Donor-Acceptor N-(Pirydyn-2-yl) Substituted Benzo(thio)amides and their Difluoroboranyl Derivatives
 J. Phys. Chem. A (IF=2.847), **120** (2016) 4116–4123 [doi](#).
358. A. D. Laurent, B. Le Guennic and D. Jacquemin*
Theoretical Spectroscopy of BASHY Dyes
 Theor. Chem. Acc. (IF=1.890), **135** (2016) 173 (8p) [doi](#).
359. S. Budzak and D. Jacquemin*
Mechanism of Fluorescence Switching in one ESIPT-Based Al³⁺ Probe
 J. Phys. Chem. B (IF=3.177), **120** (2016) 6730–6738 [doi](#).
360. M. Raoui, J. Massue*, C. Azarias, D. D. Jacquemin* and G. Ulrich*
Highly Fluorescent Extended 2-(2'-Hydroxyphenyl)Benzazole Dyes: Synthesis, Optical Properties and First-Principle Calculations
 Chem. Comm. (IF=6.319), **52** (2016) 9216–9219 [doi](#).
361. S. Nishizawa, A. Fihey, D. Jacquemin* and K. Matsuda*
Computational Investigation on the Switching Efficiency of Diarylethene: Comparison Between the First Hyperpolarizability and Exchange Interaction
 Chem. Phys. Lett. (IF=1.815), **659** (2016) 258–262 [doi](#).
362. J. Boixel*, Y. Zhu, H. Le Bozec, M. A. Benmensour, A. Boucekkine, K. Man-Chung Wong, A. Colombo, D. Roberto, V. Guerschais* and D. Jacquemin*
Contrasted Photochromic and Luminescent Properties in Dinuclear Pt(II) Complexes Linked Through a Central DTE Unit
 Chem. Comm. (IF=6.319), **52** (2016) 9833–9836 [doi](#).
363. T. Jaunet-Lahary, A. Goupille, D. Jacquemin, F. Fleury, J. Graton* and A. D. Laurent*
A Joint Theoretical and Experimental Study of the Behavior of the DIDS Inhibitor and its Derivatives
 ChemPhysChem (IF=3.075), **17** (2016) 2434–2445 [doi](#).
364. D. Jacquemin*, I. Duchemin, A. Blondel and X. Blase*
Assessment of the Accuracy of the Bethe-Salpeter (BSE/GW) Oscillator Strengths
 J. Chem. Theory Comput. (IF=5.245), **12** (2016) 3969–3981 [doi](#).
365. D. Jacquemin*
Excited-State Dipole and Quadrupole Moments: TD-DFT versus CC2
 J. Chem. Theory Comput. (IF=5.245), **12** (2016) 3993–4003 [doi](#).
366. F. Santoro* and D. Jacquemin*
Going Beyond the Vertical Approximation with TD-DFT
 WIREs Comp. Mol. Sc. (IF=14.016), **6** (2016) 460–486 [doi](#).
367. D. S. Andrianov, Y. Farré, K. J. Chen, A. Planchat, D. Jacquemin*, A. V. Cheprakov* and F. Odobel*
Trans-Substituted Benzodiazaporphyrin: a Promising Hybrid Dye Between Porphyrin and Phthalocyanine for Application in Dye-Sensitized Solar Cells
 J. Photochem. Photobiol. A: Chem. (IF=2.625), **330** (2016) 186–194 [doi](#).
368. L. Zhang, L. Favereau, Y. Farré, A. Maufroy, Y. Pellegrin, E. Blart, M. Hissler, D. Jacquemin, F. Odobel* and L. Hammarström*
Molecular-Structure Control of Electron Transfer Dynamics of Push-Pull Porphyrins as Sensitizer for NiO Based Dye Sensitized Solar Cells
 RSC Adv. (IF=3.108), **6** (2016) 77184–77194 [doi](#).



Most Read Articles

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370. P. O. Hubin*, D. Jacquemin, L. Leherte and D. P. Vercauteren
Parameterization of the ReaxFF Reactive Force Field for a Proline-Catalyzed Aldol Reaction
J. Comput. Chem. (IF=3.229), **37** (2016) 2564–2572 [doi](#).
371. R. Russo, A. Fihey, B. Mennucci* and D. Jacquemin*
Theoretical Quantification of the Modified Photoactivity of Photochromes Grafted on Metallic Nanoparticles
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372. G. Marchand*, O. Siri and D. Jacquemin*
Effects of Chemical Substitutions on the Properties of Azacalixpyrins: a First-principles Study
Phys. Chem. Chem. Phys. (IF=4.123), **18** (2016) 27308–27316 [doi](#).
373. T. T. Dang, J. F. Soulé, H. Doucet, M. A. Benmensour, A. Boucekkine, A. Colombo*, C. Dragonetti, S. Righetto, D. Jacquemin, J. Boixel* and V. Guerschais
Asymmetrical 1,3-Bis-(Heteroazolyl)Benzene Platinum Complexes 2,3 with Tunable Second-Order Nonlinear Optical Properties
Eur. J. Inorg. Chem. (IF=2.444), (2016) 4774–4782 [doi](#).
374. A. D. Laurent, E. Otten, B. Le Guennic* and D. Jacquemin*
Formazanate Boron Difluoride Dyes: Discrepancies Between TD-DFT and Wavefunction Descriptions
J. Mol. Model. (IF=1.425), **22** (2016) 263 (8p) [doi](#).
375. D. Rota Martir, G. J. Hedley, D. B. Cordes, A. M. Z. Slawin, D. Escudero, D. Jacquemin, T. Kosikova, D. Philp, D. M. Dawson, S. E. Ashbrook, I. D. W. Samuel and E. Zysman-Colman*
Exploring the Self-Assembly and Energy Transfer of Dynamic Supramolecular Iridium-Porphyrin Systems
Dalton Trans. (IF=4.029), **45** (2016) 17195–17205 [doi](#).
376. D. B. Zhang, J. Y. Wang, D. Jacquemin and Z. N. Chen*
Spectroscopic and Electrochemical Properties of Ruthenium Complexes with Photochromic Triarylamine-Dithienylethene-Acetylide Ligands
Inorg. Chem. Front. (IF=4.036), **3** (2016) 1432–1443 [doi](#).
377. D. Mendeive-Tapia*, L. Kortekaas, J. D. Steen, A. Perrier, B. Lasorne, W. R. Browne* and D. Jacquemin*
Accidental Degeneracy in the Spiropyran Radical Cation: Charge Transfer Between two Orthogonal Rings Inducing Ultra-Efficient Reactivity
Phys. Chem. Chem. Phys. (IF=4.123), **18** (2016) 31244–31253 [doi](#).
378. Z. Chen, R. Haddoub, J. Mahé, G. Marchand, D. Jacquemin*, J. Andeme-Edzang, G. Canard, D. Ferry, O. Grauby, A. Ranguis and O. Siri*
N-Substituted Azacalixpyrins: Synthesis, Properties and Self-assembly
Chem. Eur. J. (IF=5.317), **22** (2016) 17820–17832 [doi](#).
379. X. D. Jiang*, S. Li, B. Le Guennic*, D. Jacquemin, D. Escudero and L. J. Xiao
Singlet Oxygen Generation Properties of Isometrical Dibromated Thienyl-Containing Aza-BODIPYs
Phys. Chem. Chem. Phys. (IF=4.123), **18** (2016) 32686–32690 [doi](#).
380. J. Bosson, G. M. Labrador, S. Pascal, F. A. Miannay, O. Yushchenko, H. Li, L. Bouffier, N. Sojic, R. C. Tovar, G. Muller, D. Jacquemin, A. D. Laurent, B. Le Guennic, E. Vauthey* and J. Lacour*
Physicochemical and Electronic Properties of Cationic [6]Helicenes, from Chemical and Electrochemical Stabilities to Far-Red (Polarized) Luminescence
Chem. Eur. J. (IF=5.317), **22** (2016) 18394–18403 [doi](#); Err: *ibidem*, **25** (2019) 1.

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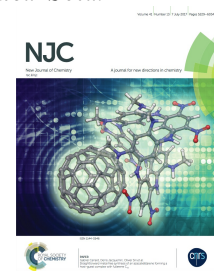


381. X. D. Jiang*, J. Guan, J. Zhao, B. Le Guennic*, D. Jacquemin, Z. Zhang, S. Chena and L. J. Xiao
Synthesis, Structure and Photophysical Properties of NIR aza-BODIPYs with -F/-N₃/-NH₂ at 1,7-Positions
Dyes Pigm. (IF=3.767), **136** (2017) 619–626 [doi](#).
382. F. Bassal, A. D. Laurent, B. Le Guennic and D. Jacquemin*
Exploring the Excited-States of Squaraine Dyes with TD-DFT, SOS-CIS(D) and ADC(2)
Dyes Pigm. (IF=3.767), **138** (2017) 169–175 [doi](#).
383. S. Pascal, S. Denis-Quanquin, C. Monnereau, A. Duperray, A. Grichine, B. Le Guennic, D. Jacquemin, J. Cuny, S. H. Chi, J. W. Perry, F. Appaix, B. van der Sanden, C. Andraud* and O. Maury*
Keto-Polymethines: a Versatile Class of Dyes with Outstanding Spectroscopic Properties for In Celulo and In Vivo Two-Photon Microscopy Imaging
Chem. Sci. (IF=9.556), **8** (2017) 381–394 [doi](#).
384. A. Fihey*, R. Russo, L. Cupellini, D. Jacquemin* and B. Mennucci*
Is Energy Transfer Limiting Multiphotochromism ? Answers from ab initio Quantification
Phys. Chem. Chem. Phys. (IF=3.906), **19** (2017) 2044–2052 [doi](#).
385. C. Azarias, I. Duchemin, X. Blase and D. Jacquemin*
Bethe-Salpeter Study of Cationic Dyes: Comparisons with ADC(2) and TD-DFT
J. Chem. Phys. (IF=2.997), **146** (2017) 034301 (8p) [doi](#).
386. D. Gao, C. Azarias, A. D'Aléo, M. Giorgi, O. Siri, T. S. Balaban, D. Jacquemin* and G. Canard*
Synthesis and Characterization of Phosphorus meso-Ester Corroles
Eur. J. Inorg. Chem. (IF=2.507), (2017) 780–788 [doi](#).
387. G. Zhang, D. Jacquemin* and D. Buccella*
Tuning the Spectroscopic Properties of Ratiometric Fluorescent Metal Indicators: Experimental and Computational Studies on Mag-fura-2 and Analogues
J. Phys. Chem. B (IF=2.923), **121** (2017) 696–705 [doi](#).
388. A. M. Grabarz, B. Jedrzejewska, A. Zakrzewska, R. Zalesny, A. D. Laurent, D. Jacquemin* and B. Osmialowski*
Photophysical Properties of Phenacylphenanthridine Difluoroboranyls: Effect of Substituent and Double Benzannulation
J. Org. Chem. (IF=4.745), **82** (2017) 1529–1537 [doi](#).
389. G. Canard*, M. Ponce-Vargas, D. Jacquemin, B. Le Guennic*, A. Felouat, E. Zaborova, A. D'Aléo and F. Fagès*
Influence of the Electron Donor Groups on the Optical and Electrochemical Properties of Boron-difluoride Complexes of Curcuminoid Derivatives: a Joint Theoretical and Experimental Study
RSC Adv. (IF=2.936), **7** (2017) 10132–10142 [doi](#).
390. A. Garcia, P. R. Pratap, C. Lüpfer, F. Cornelius, D. Jacquemin, B. Levig, T. W. Alleng and R. J. Clarke*
The Voltage-Sensitive Dye RH421 Detects a Na⁺, K⁺-ATPase Conformational Change at the Membrane Surface
BBA Biomembranes (IF=3.438), **1859** (2017) 813–823 [doi](#).
391. D. Jacquemin*, I. Duchemin, A. Blondel and X. Blase*
Benchmark of Bethe-Salpeter for Triplet Excited-States
J. Chem. Theory Comput. (IF=5.313), **13** (2017) 767–783 [doi](#).
392. D. Escudero, I. Duchemin, X. Blase and D. Jacquemin*
Modelling the Photochrome-TiO₂ Interface with Bethe-Salpeter and TD-DFT Methods
J. Phys. Chem. Lett. (IF=7.329), **8** (2017) 936–940 [doi](#).
393. D. Rota Martir, M. Averardi, D. Escudero, D. Jacquemin and E. Zysman-Colman*
Photoinduced Electron Transfer in Supramolecular Ruthenium-Porphyrin Assemblies
Dalton Trans. (IF=4.052), **46** (2017) 2255–2262 [doi](#).

394. A. Belhboub, F. Boucher, and D. Jacquemin*
Ab Initio Investigation of Photoswitches Adsorbed onto Metal Oxide Surfaces: The Case of Donor-Acceptor Stenhouse Adduct Photochromes on TiO₂ Anatase
J. Mater. Chem. C (IF=6.641), **5** (2017) 1624–1631 [doi](#).
395. C. Azarias, R. Russo, L. Cupellini, B. Mennucci* and D. Jacquemin*
Modeling Excited-State Energy Transfer in Multi-BODIPY Architectures
Phys. Chem. Chem. Phys. (IF=3.906), **19** (2017) 6443–6453 [doi](#).
396. B. Stefane*, F. Pozgan, E. Kim, E. Choi, J. C. Ribierre, J. W. Wu, M. Ponce-Vargas, B. Le Guennic*, D. Jacquemin, G. Canard, E. Zaborova, F. Fages* and A. D'Aléo*
Ethynylene-Analogues of Hemicurcuminoids: Synthesis and Ground- and Excited Properties of their Boron Difluoride Complexes
Dyes Pigm. (IF=3.767), **141** (2017) 38–47 [doi](#).
397. R. Travieso-Puente, S. Budzak, J. Chen, P. Stacko, J. T. B. H. Jastrzebski, D. Jacquemin* and E. Otten*
Arylazoindazole Photoswitches : Facile Synthesis and Functionalization via S_N-Ar Substitution
J. Am. Chem. Soc. (IF=14.357), **139** (2017) 3328–3331 [doi](#).
398. Y. M. Poronik, M. Mazur, M. Samoc*, D. Jacquemin* and D. T. Gryko*
2,5-Bis(azulenyl)pyrrolo[3,2-b]pyrroles – the Key Influence of the Linkage Position on the Linear and Non-Linear Optical Properties
J. Mater. Chem. C (IF=6.641), **5** (2017) 2620–2628 [doi](#).
399. D. Jacquemin*, I. Duchemin, and X. Blase*
Is Bethe-Salpeter Formalism Accurate for Excitation Energies ? Comparisons with TD-DFT, CASPT2 and EOM-CCSD
J. Phys. Chem. Lett. (IF=7.329), **8** (2017) 1524–1529 [doi](#).
400. S. Budzak, T. Jaunet-Lahary, A. D. Laurent, C. Laurence, M. Medved and D. Jacquemin*
Exploring the Solvatochromism of Betaine 30 with Ab Initio Tools: From Accurate Gas Phase Calculations to Implicit and Explicit Solvation Models
Chem. Eur. J. (IF=5.160), **23** (2017) 4108–4119 [doi](#).
401. J. P. Cerón-Carrasco* and D. Jacquemin
Exposing the G-Quadruplex to Electric Fields: the Role Played by Telomeres in the Propagation of DNA Errors
Phys. Chem. Chem. Phys. (IF=3.906), **19** (2017) 9358–9365 [doi](#).
402. B. Le Guennic, G. Scamani, M. J. Frisch, A. D. Laurent and D. Jacquemin*
Investigating the Optical Properties of BOIMPY Dyes with ab initio Tools
Phys. Chem. Chem. Phys. (IF=3.906), **19** (2017) 10554–10561 [doi](#).
403. C. Hierlinger, T. Roisnel, D. B. Cordes, A. M. Z. Slawin, D. Jacquemin*, V. Guerschais* and E. Zysman-Colman*
An Unprecedented Family of Luminescent Iridium(III) Complexes Bearing A six-Membered Chelated Tridentate C^NC Ligand
Inorg. Chem. (IF=4.700), **56** (2017) 5182–5188 [doi](#).
404. A. F. Henwood, J. Webster, D. Cordes, A. M. Z. Slawin, D. Jacquemin* and E. Zysman-Colman*
Phosphorescent Platinum(II) Complexes Bearing Pentafluorosulfanyl Substituted Cyclometalating Ligands
RSC Adv. (IF=2.936), **7** (2017) 25566–25574 [doi](#).
405. C. A. Guido*, G. Scamani, B. Mennucci and D. Jacquemin
Excited State Gradients for a State-Specific Continuum Solvation Approach: the Vertical Excitation Model within a Lagrangian TDDFT formulation
J. Chem. Phys. (IF=2.997), **146** (2017) 204106 (9 p) [doi](#).
406. E. Heyer, K. Benelhadj, S. Budzak, D. Jacquemin*, J. Massue* and G. Ulrich*
On the Fine-Tuning of Excited-State Intramolecular Proton Transfer (ESIPT) Process in 2-(2'-Hydroxybenzofuran)benzazole (HBBX) Dyes
Chem. Eur. J. (IF=5.160), **23** (2017) 7324–7336 [doi](#).



407. C. Azarias, M. Pawelek and D. Jacquemin*
Structural and Optical properties of Subporphyrinoids: a TD-DFT Study
J. Phys. Chem. A (IF=2.836), **121** (2017) 4306–4317 [doi](#).
408. G. Marchand*, O. Siri and D. Jacquemin*
On the Structures, Spin States, and Optical Properties of Titanium, Platinum, and Iron Azacalixphyrins: A DFT Study
Phys. Chem. Chem. Phys. (IF=3.906), **19** (2017) 15903–15913 [doi](#).
409. Y. Farré, M. Raissi, A. Fihey, Y. Pellegrin, E. Blart, D. Jacquemin* and F. Odobel*
A Blue Diketopyrrolopyrrole Sensitizer With High Efficiency in NiO Based Dye-Sensitized Solar Cells
ChemSusChem (IF=7.411), **10** (2017) 2618–2625 [doi](#).
410. Z. Chen, G. Canard,* C. Azarias, D. Jacquemin* and O. Siri*
Straightforward Metal-Free Synthesis of an Azacalix[6]arene Forming a Host-Guest Complex with Fullerene C₆₀
New. J. Chem. (IF=3.201), **41** (2017) 5284–5290 [doi](#).
411. J. Li, G. D'Avino*, A. Pershin, D. Jacquemin, I. Duchemin, D. Beljonne and X. Blase
Correlated Electron-Hole Mechanism for Molecular Doping in Organic Semiconductors
Phys. Rev. Mater. (IF=NA), **1** (2017) 025602 (9 p) [doi](#).
412. L. G. Lukaszewicz, H. Gun Ryu, A. Mikhaylov, C. Azarias, M. Banasiewicz, B. Kozankiewicz*, K. Han Ahn*, D. Jacquemin*, A. Rebane* and D. G. Gryko*
Symmetry Breaking in Pyrrolo[3,2-b]pyrroles: Synthesis, Solvatofluorochromism and Two-photon Absorption
Chem. Asian J. (IF=3.692), **12** (2017) 1736–1748 [doi](#).
413. A. Perrier* and D. Jacquemin*
Theoretical Investigation of the Photochromic Properties of [2.2]Paracyclophane-Bridged imidazole Dimers and Bis(imidazole) Dimers
Tetrahedron (IF=2.377), **73** (2017) 4936–4949 [doi](#).
414. T. Biet, T. Cauchy, Q. sun, J. Ding, A. Hauser*, P. Oulevay, T. Bürgi, D. Jacquemin, N. Vanthuyne, J. Crassous and N. Avarvari*
Luminescent Helicene-Dithiolene Platinum Diimine Complexes
Chem. Comm. (IF=6.164), **53** (2017) 9210–9213 [doi](#).
415. C. Azarias, C. Habert, S. Budzak, X. Blase, I. Duchemin and D. Jacquemin*
Calculations of $n \rightarrow \pi^$ Transition Energies: Comparisons Between TD-DFT, ADC, CC, CASPT2 and BSE/GW Descriptions*
J. Phys. Chem. A (IF=2.836), **121** (2017) 6122–6134 [doi](#).
416. J. Bednarska*, R. Zalesny*, W. Bartkowiak, B. Ośmiałowski, M. Medved and D. Jacquemin*,
Quantifying the Performances of DFT for Predicting Vibrationally Resolved Optical Spectra: Asymmetric Fluoroborate Dyes as Working Examples
J. Chem. Theory Comput. (IF=5.313), **13** (2017) 4347–4356 [doi](#).
417. W. Wang, B. Ashwood, J. Zhao*, W. Ji, D. Escudero*, D. Jacquemin* and C. Crespo-Hernandez*
Ultrafast Excited-State Dynamics in Cyclometalated Ir(III) Complexes Coordinated with Perylenebisimide and Its π -Radical Anions Ligands
J. Phys. Chem. C (IF=4.309), **121** (2017) 21184–21198 [doi](#).
418. L. Lavaud, Z. Chen, M. Elhabiri, D. Jacquemin*, G. Canard and O. Siri*
Di- vs Tetra-Substituted Quinonediimines: a Drastic Effect in Coordination Chemistry
Dalton Trans. (IF=4.052), **46** (2017) 12794–12803 [doi](#).
419. D. Rota Martir, D. Escudero, D. Jacquemin, D. B. Cordes, A. M. Z. Slawin, H. A. Fruchtl, S. L. Warriner and E. Zysman-Colman*
Homochiral Emissive Λ_8, Δ_8 -[Ir₈Pd₄]¹⁶⁺ Supramolecular Cages
Chem. Eur. J. (IF=5.160), **23** (2017) 14358–14366 [doi](#).



420. D. Jacquemin and D. Escudero*
The Short Device Lifetimes of Blue PhOLEDs: Insights into the Photostability of Blue Ir(III) Complexes
Chem. Sci. (IF=9.556), **8** (2017) 7844–7850 [doi](#).
421. C. Y. Huang, A. Bonasera, L. Hristov, Y. Garmashausen, B. M. Schmidt, D. Jacquemin* and S. Hecht*
N,N'-Disubstituted Indigos as Readily Available Red-Light Photoswitches with Tunable Thermal Half-Lives
J. Am. Chem. Soc. (IF=14.357), **139** (2017) 15205–15211 [doi](#).
422. M. Di Donato, M. M. Lerch, A. Lapini, A. D. Laurent, A. Iagatti, L. Bussoti, S. P. Ihrig, M. Medved', D. Jacquemin, W. Szymanski, W. J. Jan Buma, P. Foggi and B. L. Feringa*
Shedding Light on the Photo-Isomerization Pathway of Donor-Acceptor Stenhouse Adducts
J. Am. Chem. Soc. (IF=14.357), **139** (2017) 15596–15599 [doi](#).
423. J. P. Cerón-Carrasco* and D. Jacquemin
Tuning the Optical Properties of Phenanthriplatin: Towards new Photoactivatable Analogues
ChemPhotoChem (IF=NA), **1** (2017) 504–512 [doi](#).
424. M. Ponce-Vargas*, C. Azarias, D. Jacquemin and B. Le Guennic
A Combined TD-DFT-SOS-CIS(D) Study of BOPHY Derivatives with Potential Application in Biosensing
J. Phys. Chem. B (IF=2.923), **121** (2017) 10850–10858 [doi](#).
425. S. Budzak, G. Sciamani and D. Jacquemin*
Accurate Excited-State Geometries: a CASPT2 and Coupled-Cluster Reference Database for Small Molecules
J. Chem. Theory Comput. (IF=5.313), **13** (2017) 6237–6252 [doi](#).
426. Y. Farré, M. Raissi, A. Fihey, Y. Pellegrin, E. Blart, D. Jacquemin* and F. Odobel*
Synthesis and Properties of New Benzothiadiazole-Based Push-Pull Dyes for P-Type Dye Sensitized Solar Cells
Dyes Pigm. (IF=4.018), **148** (2018) 154–166 [doi](#).
427. E. Garoni, J. Boixel, V. Dorcet, T. Roisnel, D. Roberto, D. Jacquemin* and V. Guerschais*
Controlling the Emission in Flexibly-Linked (N⁺C⁺N)Platinum Dyads
Dalton Trans. (IF=4.052), **47** (2018) 224–232 [doi](#).
428. C. Hierlinger, H. Flint, D. B. Cordes, A. M. Z. Slawin, E. A. Gibson*, D. Jacquemin*, V. Guerschais* and Eli Zysman-Colman*
A Panchromatic, Near Infrared Ir(III) Emitter Bearing a Tripodal C⁺N⁺C Ligand as a Dye for Dye-Sensitized Solar Cells
Polyhedron (IF=2.284), **140** (2018) 109–115 [doi](#).
429. C. Azarias, L. Cupellini, A. Belhboub, B. Mennucci* and D. Jacquemin*
Modelling Excitation Energy Transfer in Covalently Linked Molecular Dyads Containing a BODIPY Unit and a Macrocyclic
Phys. Chem. Chem. Phys. (IF=3.567), **20** (2018) 1993–2008 [doi](#).
430. A. Colombo, R. Ossola, M. Magni, D. Roberto, D. Jacquemin, C. Castellano, F. Demartina* and C. Dragonetti*
Intriguing C-H...Cu Interactions in Bis-(Phenanthroline)Cu(I) Complexes: the First Example of an Anagostic Bond Between a Hydrogen Atom of a Methyl Group and Copper
Dalton Trans. (IF=4.052), **47** (2018) 1018–1022 [doi](#).
431. X. Blase*, I. Duchemin and D. Jacquemin*
The Bethe-Salpeter Equation in Chemistry: Relations with TD-DFT, Applications and Challenges
Chem. Soc. Rev. (IF=40.443), **47** (2018) 1022–1043 [doi](#).
432. M. Khelladi, N. Leclerc, D. Jacquemin, A. De Nicola* and G. Ulrich*
Synthesis and Spectral Properties of Orthogonal Red and Near IR Emitter DiBenzoBODIPYs
Tetrahedron Lett. (IF=2.259), **59** (2018) 878–881 [doi](#).



433. C. Hierlinger, A. K. Pal, F. Stella, T. Lebl, D. B. Cordes, A. M. Z. Slawin, D. Jacquemin*, V. Guerschais* and E. Zysman-Colman*
Synthesis, Characterization and Optoelectronic Properties of Iridium Complexes Bearing Non-conjugated Six-membered Chelating Ligands
Inorg. Chem. (IF=4.850), **57** (2018) 2023–2034. doi.
434. F. Forato, A. Belhboub, J. Monot, M. Petit, R. Benoit, V. Sarou-Kanian, F. Fayon, D. Jacquemin, C. Queffelec* and B. Bujoli
Phosphonate-Mediated Immobilization of Rhodium/Bipyridine Hydrogenation Catalysts
Chem. Eur. J. (IF=5.160), **24** (2018) 2457–2465 doi.
435. K. Xu, A. A. Sukhanov, Y. Zhao, J. Zhao*, W. Ji, X. Peng, D. Escudero*, D. Jacquemin and V. K. Voronkova*
Unexpected Nucleophilic Substitution Reaction of Bodipy- TEMPO Triad : Radical Enhanced Inter-system Crossing, Electron Spin Polarization and Application for Triplet-Triplet Annihilation Upconversion
Eur. J. Org. Chem. (IF=3.029), (2018) 885–895 doi.
436. D. Jacquemin*
Most Read Articles *What is the Key for Accurate Absorption and Emission Calculations, Energy or Geometry ?*
J. Chem. Theory Comput. (IF=5.313), **14** (2018) 1534–1543 doi.
437. C. A. Guido*, B. Mennucci, G. Scamamini and D. Jacquemin*
Excited State Dipole Moments in Solution: Comparison Between State-Specific and Linear-Response TD-DFT Values
J. Chem. Theory Comput. (IF=5.313), **14** (2018) 1544–1553 doi.
438. M. Ponce-Vargas, B. Stefane, Z. Zaborova, F. Fages, A. D'Aléo, D. Jacquemin* and B. Le Guennic*
Searching for New Borondifluoride- β -diketonate Complexes with Enhanced Absorption/Emission Properties Using Ab Initio Tools
Dyes Pigm. (IF=4.018), **155** (2018) 59–67 doi.
439. X. Zhang, D. Jacquemin, Q. Peng*, Z. Shuai* and D. Escudero*
Most Read Articles *A General Approach to Compute Phosphorescent OLED Efficiency*
J. Phys. Chem. C (IF=4.309), **122** (2018) 6340–6347 doi.
440. P. M. Verité, C. Azarias and D. Jacquemin*
Theoretical Spectroscopy of a NIR-absorbing Benzophthalocyanine Dye
Theor. Chem. Acc. (IF=1.598), **137** (2018) 61 (9p) doi.
441. J. Gurke, S. Budzak, B. M. Schmidt, D. Jacquemin and S. Hecht*
Efficient Light-Induced pK_a -Modulation coupled to Base-Catalyzed Photochromism
Angew. Chem. Int. Ed. (IF=12.257), **57** (2018) 4797–4801 doi.
442. D. Jacquemin and D. Escudero*
2018 PCCP HOT Articles *Thermal Equilibration Between Excited States or Solvent Effects: Unveiling the Origins of Anomalous Emissions in Heteroleptic Ru(II) Complexes*
Phys. Chem. Chem. Phys. (IF=3.567), **20** (2018) 11559–11563 doi.
443. C. Azarias, M. Ponce-Vargas, I. Navizet, P. Fleurat-Lessard, A. Romieu, B. Le Guennic, J. A. Richard*, and D. Jacquemin*
Rationalisation of the Optical Signatures of nor-Dihydroxanthene-Hemicyanine Fused Near-Infrared Fluorophores By First Principle Tools
Phys. Chem. Chem. Phys. (IF=3.567), **20** (2018) 12120–12128 doi.
444. K. G. Leslie, D. Jacquemin, E. J. New* and K. A. Jolliffe*
Expanding the Breadth of 4-Amino-1,8-Naphthalimide Photophysical Properties Through Substitution of the Naphthalimide Core
Chem. Eur. J. (IF=5.160), **24** (2018) 5569–5573 doi.
445. X. Martin-Benlloch, A. Novodomska, D. Jacquemin, E. Davioud-Charvet* and M. Elhabiri*
Iron(III) Coordination Properties of Ladanein, a Flavone Lead with a Broad-Spectrum Antiviral Activity
New. J. Chem. (IF=3.069), **42** (2018) 8074–8087 doi.

446. I. Duchemin*, C. A. Guido, D. Jacquemin and X. Blase*
The Bethe-Salpeter Formalism with Polarizable Continuum Embedding: Reconciling Linear-Response and State-Specific Features
Chem. Sci. (IF=9.556), **9** (2018) 4430–4443 [doi](#).
447. J. Rio, S. Beeck, G. Rotas, S. Ahles, D. Jacquemin, N. Tagmatarchis*, C. Ewels* and H A. Wegner*
Electronic Communication Between two [10]Cycloparaphenylenes and Bisazafullerene (C₅₉N)₂ Induced by Cooperative Complexation
Angew. Chem. Int. Ed. (IF=12.257), **57** (2018) 6930–6934 [doi](#).
448. D. Rota Martir, D. B. Cordes, A. M. Z. Slawin, D. Escudero, D. Jacquemin, S. L. Warriner and E. Zysman-Colman*
Luminescent [Ru₈Pd₄]²⁴⁺ Supramolecular Cage
Chem. Comm. (IF=6.164), **54** (2018) 6016–6019 [doi](#).
449. F. Airibi, A. Panossian, D. Jacquemin, J. P. Vors, S. Pazenok, D. R. Leroux* and M. Elhabiri*
A Physico-chemical Investigation on Fluorine-Enriched Quinolines
New J. Chem. (IF=3.069), **42** (2018) 10036–10047 [doi](#).
450. Z. Hong, E. Garoni, A. Colombo, C. Dragonetti*, D. Marinotto, S. Righetto, D. Roberto, D. Jacquemin*, J. Boixel* and V. Guerschais
para-Substituted-1,3-di(2-pyridyl)benzene Platinum(II) Complexes: Photo-modulation of Luminescence and Second-order Nonlinear Optical Properties
Inorg. Chem. (IF=4.850), **57** (2018) 7051–7063 [doi](#).
451. C. Hierlinger, D. Cordes, A. M. Z. Slawin, A. Colombo, C. Dragonetti*, S. Righetto, D. Roberto, D. Jacquemin*, E. Zysman-Colman* and V. Guerschais
An Investigation on the Second-Order Nonlinear Optical Response of Cationic Bipyridine or Phenanthroline Iridium(III) Complexes Bearing Cyclometallated 2-Phenylpyridines with a Triphenylamine Substituent
Dalton Trans. (IF=4.052), **47** (2018) 8292–8300 [doi](#).
452. H. G. Ruy, M. F. Mayther, J. Tamayo, C. Azarias, E. M. Espinoza, M. Banasiewicz, L. Lukasiewicz, Y. M. Poronik, A. Jezewski, Y. M. Poronik, J. Clark, J. B. Derr K. H. Ahn*, D. T. Gryko*, D. Jacquemin* and V. I. Vullev*
Bidirectional Solvatofluorochromism of a Pyrrolo[3,2-b]pyrrole-diketopyrrolopyrrole Hybrid
J. Phys. Chem. C (IF=4.309), **122** (2018) 13424–13434 [doi](#).
453. D. Rota Martir, A. Pizzolante, D. Escudero, D. Jacquemin*, S. L. Warriner and E. Zysman-Colman*
Photoinduced Energy and Electron Transfer Between a Photoactive Cage Based on a Thermally Activate Delayed Fluorescence Ligand and Encapsulated Fluorescent Dyes
ACS Appl. Energy Mater. (IF=N/A, 2019 FI=4.473), **1** (2018) 2971–2978 [doi](#).
454. L. Kortekaas, J. Chen, D. Jacquemin,* and W. R. Browne*
Proton Stabilized Photochemically Reversible E/Z Isomerization of Spiropyrans
J. Phys. Chem. B (IF=2.923), **122** (2018) 6423–6430 [doi](#).
455. E. Bremond, M. Savarese, C. Adamo* and D. Jacquemin*
Accuracy of TD-DFT Geometries: a Fresh Look
J. Chem. Theory Comput. (IF=5.313), **14** (2018) 3715–3727 [doi](#).
456. A. Scemama, A. Benali, D. Jacquemin, M. Caffarel and P. F. Loos*
Excitation Energies from Diffusion Monte Carlo Using Selected Configuration Interaction Nodes
J. Chem. Phys. (IF=2.997), **149** (2018) 034108 (8 p) [doi](#).
457. S. Gauthier*, A. Porter, S. Achelle, T. Roisnel, V. Dorcet, A. Barsella, N. Le Poul, P. Guevara Level, D. Jacquemin and F. Robin-Le Guen
Mono- and Diplatinum Polyynediyl Complexes as Potential Push-Pull Chromophores: Synthesis, Characterization, TD-DFT Modeling, Photophysical and NLO properties
Organometallics (IF=4.100), **37** (2018) 2232–2244 [doi](#).
458. C. Azarias, S. Pascal, O. Siri* and D. Jacquemin*
Central Substitution of Azacalixpyrins: a Strategy Towards Acidochromic NIR Dyes
Phys. Chem. Chem. Phys. (IF=3.567), **20** (2018) 20056–20069 [doi](#).

459. P. F. Loos, N. Galland and D. Jacquemin*

Most Read Articles

Theoretical 0-0 Energies with Chemical Accuracy
J. Phys. Chem. Lett. (IF=7.329), **9** (2018) 4646–4651 [doi](#).

460. J. Massue*, D. Jacquemin* and G. Ulrich*

Molecular Engineering of Excited-State Intramolecular Proton Transfer (ESIPT) Dual and Triple Emitters
Chem. Lett. (IF=1.485), invited review, **47** (2018) 1083–1089 [doi](#).

461. B. Jedrzejewska, A. Skotnicka, A. D. Laurent, M. Pietrzak, D. Jacquemin* and B. Osmialowski*

The Influence of the Nature of the Amino Group in Highly Fluorescent Difluoroborates Exhibiting Intramolecular Charge Transfer
J. Org. Chem. (IF=4.745), **83** (2018) 7779–7788 [doi](#).

462. J. Massue*, A. Felouat, P. M. V  rit  , D. Jacquemin*, K. Cyprych, M. Durko, L. Sznitko, J. Mysliwiec* and G. Ulrich*

Extended Excited-State Intramolecular Proton Transfer (ESIPT) Emitter for Random Lasing Application
Phys. Chem. Chem. Phys. (IF=3.567), **20** (2018) 19958–19963 [doi](#).

463. C. Hierlinger, D. B. Cordes, A. M. Z. Slawin, D. Jacquemin*, V. Guerschais* and E. Zysman-Colman*

Phosphorescent Iridium Complexes Bearing a Nonconjugated Six-Membered Chelating Ring Ancillary Ligand: Tuning Emission Color Towards the Blue
Dalton Trans. (IF=4.052), **47** (2018) 10569–10577 [doi](#).

464. P. F. Loos*, A. Scemama, A. Blondel, Y. Garniron, M. Caffarel and D. Jacquemin*

Most Read Articles

A Mountaineering Strategy to Excited States: Highly-Accurate Reference Energies and Benchmarks
J. Chem. Theory Comput. (IF=5.313), **14** (2018) 4360–4379 [doi](#).

465. S. Pascal*, L. Lavaud, C. Azarias, G. Canard, M. Giorgi, D. Jacquemin* and O. Siri*

Controlling the Canonical/Zwitterionic Balance through Intramolecular Proton Transfer: a Strategy for Vapochromism
Mater. Chem. Front. (IF=N/A, 2019 FI=6.788), **2** (2018) 1618–1625 [doi](#).



466. Q. Huauilm  , A. Sutter, S. Fall, D. Jacquemin*, P. L  v  que, P. Retaill  au, N. Leclerc* and G. Ulrich*

Versatile Synthesis of α -fused BODIPY Displaying Intense Absorption in the NIR and High Electron Affinity
J. Mater. Chem. C (IF=6.641), **6** (2018) 9925–9931 [doi](#).



467. S. Budzak and D. Jacquemin*

Excited State Intramolecular Proton Transfer in Julolidine Derivatives: an ab initio Study
Phys. Chem. Chem. Phys. (IF=3.567), **20** (2018) 25031–25038 [doi](#).

468. Z. Chen, G. Canard, D. Jacquemin*, C. Bucher, M. Giorgi, and O. Siri*

Heterobimetallic Effect as a new Route to Access Multinuclear Complexes
Inorg. Chem. (IF=4.850), **57** (2018) 12536–12542 [doi](#).

469. L. Lavaud, S. Pascal*, K. Metwally, D. Gasteau, A. Da Silva*, Z. Chen, M. Elhabiri, G. Canard, D. Jacquemin and O. Siri*

Azacalixphyryns as NIR Photoacoustic Contrast Agents
Chem. Comm. (IF=6.164), **54** (2018) 12365–12368 [doi](#).

470. L. Leherte*, A. Petit, D. Jacquemin, D. P. Vercauteren and A. D. Laurent

Investigating Cyclic Peptides Inhibiting CD2-CD58 Interactions through Molecular Dynamics and Molecular Docking Methods
J. Comput. Aided Mol. Des. (IF=3.250), **32** (2018) 1295–1313 [doi](#).

471. K. Gutkowski, C. Azarias, B. Kozankiewicz*, D. Jacquemin* and D. T. Gryko*

Synthesis and Photophysical Properties of N-Arylated Diketopyrrolopyrroles
Eur. J. Org. Chem. (IF=3.029), (2018) 6643–6648 [doi](#).

472. J. Massue*, A. Felouat, M. Curtil, P. M. Vérité, D. Jacquemin* and G. Ulrich*
Solution and Solid-State Excited-State Intramolecular Proton Transfer (ESIPT) Emitters Incorporating Bis-trialkyl- or Triarylsilyl ethynyl Units
Dyes Pigm. (IF=4.613), **160** (2019) 915–922 [doi](#).
473. F. Barakat, M. Vansteelandt, A. Triastuti, P. Jargeat, D. Jacquemin, J. Graton, K. Mejia, B. Cabanillas, L. Vendier, M. Haddad and N. Fabre*
Bisthiodiketopiperazines with Two Spirocyclic Centers from Lipstick tree derived Endophytic Fungus Botryosphaeria mamane
Phytochemistry (IF=3.044), **158** (2019) 142–148 [doi](#).
474. D. Jacquemin*, M. Khelladi, A. De Nicola and G. Ulrich*
Turning ESIPT-Based Triazine Fluorophores into Dual Emitters: from Theory to Experiment
Dyes Pigm. (IF=4.613), **163** (2019) 475–482 [doi](#).
475. M. Tasior, G. Clermont, M. Blanchard-Desce*, D. Jacquemin* and D. T. Gryko*
Synthesis of Bis(arylethynyl)pyrrolo[3,2-b]pyrroles and an Effect of Intramolecular Charge-transfer on Their Photophysical Behavior
Chem. Eur. J. (IF=4.857), **25** (2019) 598–608 [doi](#).
476. L. Abad Galan, D. B. Bordes, A. M. Z. Slawin, D. Jacquemin*, M. I. Ogden*, M. Massi* and E. Zysman-Colman*
Analyzing the Relation Between Structure and Aggregation Induced Emission (AIE) Properties of Iridium(III) Complexes through Modification of Non-Chromophoric Ancillary Ligands
Eur. J. Inorg. Chem. (IF=2.529), (2019) 152–163 [doi](#).
477. R. Boyaala, R. Touzani, T. Roisnel, V. Dorcet, E. Caytan, D. Jacquemin*, J. Boixel*, V. Guerschais*, H. Doucet* and J.F. Soulé*
Catalyst-Controlled Regiodivergent C-H Arylation of Fluorinated 2-Arylpyridines and 2-Arylquinolines: Preparation of Luminescent Iridium Complexes
ACS Catal. (IF=12.350), **9** (2019) 1320–1328 [doi](#).
478. P. M. Vérité, C. A. Guido and D. Jacquemin*
First-Principle Investigation of the Double ESIPT Process in a Thiophene-Based Dye
Phys. Chem. Chem. Phys. (IF=3.430), **21** (2019) 2307–2317 [doi](#).
479. S. Pascal*, L. Lavaud, C. Azarias, A. Varlot, G. Canard, M. Giorgi, D. Jacquemin* and O. Siri*
Azacalixquinarenes: from Canonical to (Poly-)Zwitterionic Macrocycles through Intramolecular H-Transfer
J. Org. Chem. (IF=4.335), **84** (2019) 1387–1397 [doi](#).
480. M. Munch, M. Curtil, P. M. Vérité, D. Jacquemin*, J. Massue* and G. Ulrich*
Ethynyl-Tolyl Extended 2-(2'-Hydroxyphenyl)benzoxazole Dyes: Solution and Solid-state Excited-State Intramolecular Proton Transfer (ESIPT) Emitters
Eur. J. Org. Chem. (IF=2.889), (2019) 1134–1144 [doi](#).
481. J. P. Cerón-Carrasco* and D. Jacquemin
i-Motif DNA Structures Upon Electric Field Exposure: Completing the Map of Induced Genetic Error
Theor. Chem. Acc. (IF=1.498), **138** (2019) 35 (6 p) [doi](#).
482. P. F. Loos*, M. Boggio-Pasqua, A. Scemana, M. Caffarel and D. Jacquemin
Reference Energies for Double Excitations
J. Chem. Theory Comput. (IF=5.011), **15** (2019) 1939–1956 [doi](#).
483. A. Daher, D. Jacquemin, V. Guerschais*, J.F. Soulé* and H. Doucet*
Reactivity of 4-Phenylthiazoles in Ruthenium Catalyzed Direct Arylations
Appl. Organometal. Chem. (IF=3.140), **33** (2019) e4794 (11p) [doi](#).
484. P. F. Loos and D. Jacquemin*
Chemically Accurate 0-0 Energies with not-so-Accurate Excited State Geometries
J. Chem. Theory Comput. (IF=5.011), **15** (2019) 2481–2491 [doi](#).

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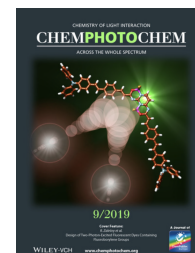
2019 PCCP HOT Articles

Most Read Articles



485. S. Zheng, G. Lingyue, M. J. Hsien Ong, D. Jacquemin, A. Romieu*, J. A. Richard* and R. Srinivasan* *Divergent synthesis of 5',7'-Difluorinated Dihydroxanthene-Hemicyanine Fused Near-Infrared Fluorophores* Org. Biol. Chem. (IF=3.412), **17** (2019) 4291–4300 doi.
486. R. Haldar, A. Mazel, M. Krstic, Q. Zhang, M. Jakoby, I. A. Howard, B. S. Richards, N. Jung, D. Jacquemin, S. Diring* W. Wenzel* F. Odobel* and C. Wöll* *A de novo Strategy for Predictive Crystal Engineering to Tune Excitonic Coupling* Nature Commun. (IF=12.121), **10** (2019) 2048 (7 p) doi.
487. G. Bretel, E. Le Grogne, D. Jacquemin, T. Hirose, K. Matsuda and F.X. Felpin* *Fabrication of Robust Spatially-Resolved Photochromic Patterns on Cellulose Papers by Covalent Printing* ACS Appl. Polym. Mater. (IF=N/A, 2019 FI=4.089), **1** (2019) 1240–1250 doi.
488. A. Grabarz, B. Jedrzejewska, A. Skotnicka, N. Arul Murugan, F. Patalas, W. Bartkowiak, D. Jacquemin* and B. Osmialowski* *The Impact of the Heteroatom in Five-Membered Ring on the Photophysical Properties of Difluoroborates* Dyes Pigm. (IF=4.613), **170** (2019) 170481 (12 p) doi.
489. M. Katari, D. Carmichael, D. Jacquemin and G. Frison* *Structure of Electronically Reduced N-Donor Bidentate Ligands and their Heteroleptic Four-coordinate Zinc Complexes: a Survey of DFT Results* Inorg. Chem. (IF=4.825), **58** (2019) 7169–7179 doi.
490. S. Golten, A. Patinec, J. Rocher, K. Akoumany, J. Graton, D. Jacquemin, J. Y. Le Questel, A. Tessier, J. Lebreton, V. Blot, M. Pipelier, J. Le Pendu, B. Linclau* and D. Dubreuil* *3,4-Dideoxy-3,3,4,4-tetrafluoro- and 4-OH Epimeric 3-Deoxy-3,3-difluoro- α -GalCer Analogues: Synthesis and Biological Evaluation on Human iNKT Cells Stimulation* Eur. J. Med. Chem. (IF=5.572), **178** (2019) 195–213 doi.
491. A. Scemama, M. Caffarel, A. Benali, D. Jacquemin and P. F. Loos* *Influence of Pseudopotentials on Excitation Energies From Selected Configuration Interaction and Diffusion Monte Carlo* Res. Chem. (IF=N/A), **1** (2019) 100002 (7 p) doi.
492. F. Legalite, D. Escudero, Y. Pellegrin, E. Blart, D. Jacquemin and F. Odobel* *“Iridium Effect” in Cyclometalated Iridium Complexes for p-Type Dye Sensitized Solar Cells* Dyes Pigm. (IF=4.613), **171** (2019) 107693 (10 p) doi.
493. J. Massue*, T. Pariat, P. M. V  rit  , D. Jacquemin*, M. Durko, L. Sznitko, J. Mysliwiec* and G. Ulrich* *Natural Born Laser Dyes: Excited-State Intramolecular Proton Transfer (ESIPT) Emitters and their use in Random Lasing Studies* Nanomaterials (IF=4.324), **9** (2019) 1093 (13 p) doi.
494. P. M. V  rit  , S. H  d   and D. Jacquemin* *A Theoretical Elucidation of the Mechanism of Tuneable Fluorescence in a Full-Colour Emissive ESIPT Dye* Phys. Chem. Chem. Phys. (IF=3.430), **21** (2019) 17400–17409 doi.
495. S. Gauthier*, F. Robin-Le Guen, L. Wojcik, N. Le Poul, A. Planchat, Y. Pellegrin*, P. Guevara-Level, N. Szuwarski, M. Boujtita, D. Jacquemin* and F. Odobel* *Synthesis and Properties of Novel Pyranilidene-Based Organic Sensitizers for Dye-Sensitized Solar Cells* Dyes Pigm. (IF=4.613), **171** (2019) 107747 (10p) doi.
496. C. Suellen, R. Garcia Freitas, P. F. Loos and D. Jacquemin* *Cross Comparisons Between Experiment, TD-DFT, CC, and ADC for Transition Energies* J. Chem. Theory Comput. (IF=5.011), **15** (2019) 4581–4590 doi.

497. M. Banasiewicz, R. Stezycki, G. D. Kumar, M. Krzeszewski, M. Tasior, B. Koszarna, A. Janiga, O. Vakuliuk, B. Sadowski, D. T. Gryko* and D. Jacquemin*
Electronic Communication in Pyrrolo[3,2-b]Pyrroles Possessing Sterically Hindered Aromatic Substituents
Eur. J. Org. Chem. (IF=2.889), (2019) 5247–5253 [doi](#).
498. M. Tasior, B. Koszarna, D. C. Young, B. Bernard, D. Jacquemin*, D. Gryko* and D. T. Gryko*
Fe³⁺ Catalyzed Synthesis of Pyrrolo[3,2-b]Pyrroles: Formation of New Dyes and Photophysical Studies
Org. Chem. Front. (IF=5.155), **6** (2019) 2939–2948 [doi](#).
499. P. F. Loos and D. Jacquemin*
Evaluating 0-0 Energies with Theoretical Tools: a Short Review
ChemPhotoChem (IF=2.838), **3** (2019) 684–696 [doi](#).
500. R. Zalesny*, N. Szczotka, A. Grabarz, B. Osmialowski and D. Jacquemin*
Design of Two-Photon-Excited Fluorescent Dyes Containing Fluoroborylene Groups
ChemPhotoChem (IF=2.838), **3** (2019) 719–726 [doi](#).
501. S. Pascal, Q. Bellier, S. David, P. A. Bouit, S. H. Chi, N. S. Makarov, B. Le Guennic, S. Chibani, G. Berginc, P. Feneyroux, D. Jacquemin*, J. W. Perry, O. Maury* and C. Andraud*
Unraveling the Two-Photon Absorption and Excited State Absorption of Aza-BODIPY Dyes for Optical Power Limiting in the SWIR band
J. Phys. Chem. C (IF=4.189), **123** (2019) 23661–23673 [doi](#).
502. P. Guevara-Level, S. Pascal, O. Siri* and D. Jacquemin*
First Principles Investigation of the Spectral Properties of Neutral, Zwitterionic, and bis-Cationic Azaacenes
Phys. Chem. Chem. Phys. (IF=3.430), **21** (2019) 22910–22918 [doi](#).
503. A. Fihey* and D. Jacquemin*
Performances of Density Functional Tight-Binding Methods for Describing Ground and Excited State Geometries of Organic Molecules
J. Chem. Theory Comput. (IF=5.011), **15** (2019) 6267–6276 [doi](#).
504. P. L. dos Santos, D. Chen, P. Rajamalli, T. Matulaitis, D. B. Cordes, A. M. Z. Slawin, D. Jacquemin, E. Zysman-Colman* and I. D. W. Samuel*
The use of Pyrimidine and Pyrazine Bridges as a Design Strategy to Improve the Performance of Thermally Activated Delayed Fluorescence Organic Light Emitting Diodes
ACS Appl. Mat. Inter. (IF=8.758), **11** (2019) 45171–45179 [doi](#).
505. G. Tang, A. A. Sukhanov, J. Zhao*, X. Li, W. Yang, Z. Wang, Liu, Q., V. K. Voronkova*, M. Di Donato*, D. Escudero* and D. Jacquemin*
Red Thermally-Activated Delayed Fluorescence and Intersystem Crossing in Compact Naphthalimide-Phenothiazine Electron Donor/Acceptor Dyads
J. Phys. Chem. C (IF=4.189), **123** (2019) 30171–30186 [doi](#).
506. D. Rota Martir, L. Delforce, D. B. Cordes, A. M. Z. Slawin, S. L. Warriner, D. Jacquemin and E. Zysman-Colman*
A Pd₃L₆ Supramolecular Cage Incorporating Photoactive [2.2]Paracyclophane Units
Inorg. Chem. Front. (IF=6.569), **7** (2020) 232–238 [doi](#).
507. A. Chrayteh, C. Ewels* and D. Jacquemin*
Dual Fluorescence in Strap ESIPT Systems: A Theoretical Study
Phys. Chem. Chem. Phys. (IF=3.676), **22** (2020) 854–863 [doi](#).
508. L. Lavaud, C. Azarias, G. Canard*, S. Pascal, J. Galiana, M. Giorgi, Z. Chen, D. Jacquemin* and O. Siri*
Fused Bis-Azacalixpyrin that Reaches NIR-II Absorption
Chem. Comm. (IF=6.222), **56** (2020) 896–899 [doi](#).



509. P. F. Loos* and D. Jacquemin*
Is ADC(3) as Accurate as CC3 for Valence and Rydberg Transition Energies?
J. Phys. Chem. Lett. (IF=6.475), **11** (2020) 974–980 [doi](#).
510. L. Cupellini*, D. Calvani, D. Jacquemin and B. Mennucci*
Charge Transfer from the Carotenoid can Quench Chlorophyll Excitation in Antenna Complexes of Plants
Nature Commun. (IF=14.919), **11** (2020) 662 (8p) [doi](#).
511. R. Duwald, J. Bosson, S. Pascal, S. Grass, F. Zinna, C. Besnard, L. Di Bari, D. Jacquemin* and J. Lacour*
Merging Polyacenes and Cationic Helicenes: from Weak to Intense Chiroptical Properties in the Far Red Region
Chem. Sci. (IF=9.825), **11** (2020) 1165–1169 [doi](#).
512. P. F. Loos*, F. Lippirani*, M. Boggio-Pasqua, A. Scemama and D. Jacquemin*
A Mountaineering Strategy to Excited States: Highly-Accurate Energies and Benchmarks for Medium Size Molecules
J. Chem. Theory Comput. (IF=6.006), **16** (2020) 1711–1741 [doi](#).
513. P. F. Loos*, A. Scemama and D. Jacquemin*
The Quest For Highly Accurate Excitation Energies: A Computational Perspective
J. Phys. Chem. Lett. (IF=6.475), invited perspective, **11** (2020) 2374–2383 [doi](#).
514. K. Gutkowski, K. Skonieczny, M. Bugaj, D. Jacquemin* and D. T. Gryko*
First Method for N-Arylation of Diketopyrrolopyrroles with Aryl Triflates
Chem. Asian J. (IF=4.568), **15** (2020) 1369–1375 [doi](#).
515. P. F. Loos*, A. Scemama, I. Duchemin, D. Jacquemin* and X. Blase*
Pros and Cons of the Bethe-Salpeter Formalism for Ground-State Energies
J. Phys. Chem. Lett. (IF=6.475), **11** (2020) 3536–3545 [doi](#).
516. S. Gauthier*, F. Robin-Le Guen, L. Wojcik, N. Le Poul, A. Planchat, Y. Pellegrin*, P. Guevara-Level, N. Szuwarski, M. Boujtita, D. Jacquemin* and F. Odobel*
Comparative Studies of New Pyranylidene-Based Sensitizers Bearing Single or Double Anchoring Groups for Dye-Sensitized Solar Cells
Solar Energy (IF=5.742), **205** (2020) 310–319 [doi](#).
517. P. F. Loos*, A. Scemama, M. Boggio-Pasqua and D. Jacquemin*
A Mountaineering Strategy to Excited States: Highly-Accurate Energies and Benchmarks for Exotic Molecules and Radicals
J. Chem. Theory Comput. (IF=6.006), **16** (2020) 3720–3736 [doi](#).
518. D. C. Young, M. Tasior, A. D. Laurent, L. Dobrzycki, M. K. Cyranski, N. Tkachenko*, D. Jacquemin* and D. T. Gryko*
Photostable Orange-Red Emitting Unsymmetrical Diketopyrrolopyrrole-BODIPY Hybrids
J. Mater. Chem. C (IF=7.393), **8** (2020) 7708–7717 [doi](#).
519. L. G. Lukasiewicz, M. Rammo, C. Stark, M. Krzeszewski, D. Jacquemin*, A. Rebane* and D. T. Gryko*
Ground and Excited State Symmetry Breaking and Solvatofluorochromism in Centrosymmetric Pyrrolo[3,2-b]pyrroles Possessing two Nitro Groups
ChemPhotoChem (IF=3.849), **4** (2020) 508–519 [doi](#).
520. T. Delouche, A. Vacher, E. Caytan, T. Roisnel, B. Le Guennic, D. Jacquemin*, M. Hissler and P. A. Bouit*
Multi-Stage Redox Systems Based on Dicationic P-Containing Polycyclic Aromatic Hydrocarbons
Chem. Eur. J. (IF=5.236), **26** (2020) 8226–8229 [doi](#).
521. B. Osmiamlowski*, E. F. Petrushevich, M. A. Antoniuk, I. Grela, M. A. Bin Jassar, M. Nyk, J. M. Luis, B. Jedrzejewska, R. Zalesny and D. Jacquemin*
Controlling Two-Photon Action Cross Section by Changing a Single Heteroatom Position in Fluorescent Dyes
J. Phys. Chem. Lett. (IF=6.475), **11** (2020) 5920–5925 [doi](#)

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522. L. Favereau*, C. Quinton, C. Poriél, T. Roisnel, D. Jacquemin and J. Crassous
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J. Phys. Chem. Lett. (IF=6.475), **11** (2020) 6426–6434 [doi](#).
523. Z. Chen, K. Lhoussain, C. Bucher, D. Jacquemin*, D. Luneau and O. Siri*
Unconventional Access to Solvatochromic Nickel(II) Dyes Featuring a Coordination-Induced Spin Crossover Behavior
Dyes Pigm. (IF=4.889), **183** (2020) 108645 (7 p) [doi](#).
524. M. Trinel, A. C. Le Lamer*, V. Jullian, D. Jacquemin, J. Graton, V. Cristofoli, E. Crossay, M. Yassine, N. Vergnolle, B. J. Cabanillas, C. Racaud-Sultan* and N. Fabre
Daphnanes Diterpenes from Hura Crepitans L. and Activity Against Human Colorectal Cancer Cells Caco-2
Bioorg. Chem. (IF=5.275), **103** (2020) 104132 (13 p) [doi](#).
525. L. Adair, N. Trinh, P. M. Vérité, D. Jacquemin, K. Jolliffe and E. New*
Synthesis of Aryl-Nitro Functionalised 4-Amino-1,8-Naphthalimides and Their Evaluation as Fluorescent Hypoxia Sensors
Chem. Eur. J. (IF=5.236), **26** (2020) 10064–10071 [doi](#).
526. L. Kortekaas, J. D. Steen, D. R. Duijnste, D. Jacquemin* and W. R. Browne*
Non-Commutative Switching of Double Spiropyrans
J. Phys. Chem. A (IF=2.781), **124** (2020) 6458–6467 [doi](#).
527. L. Norel*, K. Bernot, F. Gendron, C. A. Gould, T. Roisnel, S. Delbaere, B. Le Guennic, D. Jacquemin, and S. Rigaut.
Coordination-Enhanced Photochromism in Dysprosium Dinuclear Complexes with Photomodulated Single-Molecule Magnet Behavior
Chem. Sq. (IF=NA), **4** (2020) 2 (16 p) [doi](#).
528. X. Blase*, I. Duchemin, D. Jacquemin and P. F. Loos*
Bethe-Salpeter Equation Formalism: From Physics to Chemistry
J. Phys. Chem. Lett. (IF=6.475), *invited perspective*, **11** (2020) 7371–7382 [doi](#).
529. K. Skonieczny, I. Papadopoulos, D. Thiel, K. Gutkowski, P. Haines, P. M. McCosker, A. D. Laurent, P. A. Keller, T. Clark, D. Jacquemin*, D. M. Guldi* and D. T. Gryko*
How to Make Nitroaromatics Glow: Next Generation Large, χ -Shaped, Centrosymmetric Diketopyrrolopyrroles
Angew. Chem. Int. Ed. (IF=15.336), **59** (2020) 16104–16113 [doi](#).
530. T. R. Rusch, A. Schlimm, N. R. Krekielehn, T. Tellkamp, S. Budzak, D. Jacquemin, F. Tuczek, R. Herges and O. M. Magnussen*
Observation of Collective Photoswitching in Free-Standing TATA-based Azobenzenes on Au(111)
Angew. Chem. Int. Ed. (IF=15.336), **59** (2020) 17192–17196 [doi](#).
531. M. R. Koli, A. Labiod, S. Chakarborty, M. Kumar, P. Lévêque*, G. Ulrich, N. Leclerc, D. Jacquemin* and S. Mula*
Tuning the Emission Color of Indolo[3,2-b]carbazole based Boron Complexes and their Application in OFET and Bioimaging
ChemPhotoChem (IF=3.849), **4** (2020) 729–741 [doi](#).
532. N. Saleh, A. Bosmani, C. Besnard, T. Bürgi, D. Jacquemin* and J. Lacour*
Simple Access to Novel Chiral Rigid Hemicyanine Fluorophores from Tröger Bases and α -Imino Carbenes
Org. Lett. (IF=6.005), **22** (2020) 7599–7603 [doi](#).
533. P. Liesfeld, Y. Garmshausen, S. Budzak, J. Becker, A. Dallmann, D. Jacquemin* and S. Hecht*
Highly Cooperative Photoswitching in Dihydropyrene Dimers
Angew. Chem. Int. Ed. (IF=15.336), **59** (2020) 19352–19358 [doi](#).

534. H. V. Tran, H. D. Vu, J. Graton, D. Jacquemin, J. Renault and P. Uriac*
Synthesis of Heterocyclic Enamine-Zinc Complexes as Precursors of Stereocontrolled Substitution of Nitrogen α -Position
Tetrahedron Lett. (IF=2.415), **61** (2020) 152405 (4 p) [doi](#).
535. A. Torres Ruiz, M. H. E. Bousquet, S. Pascal*, G. Canard, M. Elhabiri, D. Jacquemin* and O. Siri*
Small Panchromatic and NIR Absorbers from Quinoid Zwitterions and Cations
Org. Lett. (IF=6.005), **22** (2020) 7997–8001 [doi](#).
536. L. Lavaud, C. Azarias, G. Canard, S. Pascal*, D. Jacquemin* and O. Siri*
Pointing Out One Tautomer: Synthesis, Spectroscopic and Theoretical Investigation of a Mixed N-Aryl/Alkyl Substituted Near-Infrared Azacalixphyrin
New. J. Chem. (IF=3.591), **44** (2020) 18130–18137 [doi](#).
537. S. David, D. Chateau, H. J. Chang, L. Karlsson, M. V. Bondar, C. Lopes, B. Le Guennic, D. Jacquemin, G. Berginc, O. Maury*, S. Parola* and C. Andraud*
High Performance Optical Power Limiting Filters at Telecommunication Wavelengths: when azabodipy dyes bond to sol-gel materials
J. Phys. Chem. C (IF=4.126), **124** (2020) 24344–24350 [doi](#).
538. A. Chrayteh, C. Ewels* and D. Jacquemin*
TD-DFT and CC2 Insights into the Dual-Emissive Behavior of 2-(2'-Hydroxyphenyl)oxazoles Core and their Derivatives
Phys. Chem. Chem. Phys. (IF=3.676), **22** (2020) 25066–25074 [doi](#).
539. L. N. Lameijer, S. Budzak, N. A. Simeth, M. J. Hansen, B. L. Feringa, D. Jacquemin* and W. Szymanski*
General Principles for the Design of Visible-Light-Responsive Photoswitches: Tetra-ortho-Chloro-Azobenzenes
Angew. Chem. Int. Ed. (IF=15.336), **59** (2020) 21663–21670 [doi](#).
540. T. Delouche, A. Vacher, T. Roisnel, M. Cordier, J. F. Audibert, B. Le Guennic, F. Miomandre*, D. Jacquemin*, M. Hissler and P. A. Bouit*
Luminescent Molecular Switches Based on Dicationic P-doped Polycyclic Aromatic Hydrocarbons
Mater Adv. (IF=N/A), **1** (2020) 3369–3377 [doi](#).
541. A. Chrayteh, A. Blondel, P. F. Loos and D. Jacquemin*
A Mountaineering Strategy to Excited States: Highly-Accurate Oscillator Strengths and Dipole Moments of Small Molecules
J. Chem. Theory Comput. (IF=6.578), **17** (2021) 416–438 [doi](#).
542. J. F. Longevial, Z. Chen, S. Pascal, D. Jacquemin* and O. Siri*
Stabilization of a 12- π Electrons Diamino-Benzoquinonediimine Tautomer
Chem. Comm. (IF=6.065), **57** (2021) 548–551 [doi](#).
543. O. D. C. De Azevedo*, P. I. P. Elliott*, C. D. Gabbutt, B. M. Heron*, D. Jacquemin*, C. R. Rice and P. A. Scattergood
Quenching of the Phosphorescence of Thermally Reversible Photochromic Naphthopyran Re(I) Complexes Initiated by either Visible or Ultraviolet Radiation
Dalton Trans. (IF=4.569), **50** (2021) 830–834 [doi](#).
544. R. Sarkar, M. Boggio-Pasqua, P. F. Loos* and D. Jacquemin*
Benchmarking TD-DFT and Wave Function Methods for Oscillator Strengths and Excited-State Dipole Moments
J. Chem. Theory Comput. (IF=6.578), **17** (2021) 1117–1132 [doi](#).
545. T. Pariat, M. Munch, M. Durko, J. Mysliwiec, P. Retailleau, P. M. V  rit  , D. Jacquemin*, J. Massue* and G. Ulrich*
Impact of Heteroatom Substitution on Dual-State Emissive Rigidified 2-(2'-hydroxyphenyl)benzazole Dyes: Towards Ultra-Bright ESIPT Fluorophores
Chem. Eur. J. (IF=5.020), **27** (2021) 3483–3495 [doi](#).

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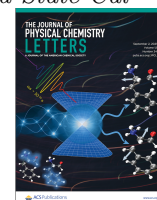
546. S. David, H. J. Chang, C. Lopez, B. Le Guennic, G. Berginc, E. van Stryland, M. V. Bondar, D. Hagan, D. Jacquemin*, C. Andraud* and O. Maury*
Benzothiadiazole Substituted aza-BODIPY Dyes: Two-Photon Absorption Enhancement for Improved Optical Limiting Performances at Telecommunication Wavelengths
Chem. Eur. J. (IF=5.020), **27** (2021) 3517–3525 doi.
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High-field and Benchtop NMR Spectroscopy for the Characterization of New Psychoactive Substances
Forensic Sci. Int. (IF=2.676), **21** (2021) 110718 (8 p) doi.
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Switch-On Optical Chemosensors for Lithium Ions Based on the Diketopyrrolopyrrole Chromophore
Chem. Asian J. (IF=4.839), **16** (2021) 355–362 doi.
549. M. V  ril, A. Scemama, M. Caffarel, F. Lipparini, M. Boggio-Pasqua, D. Jacquemin* and P. F. Loos*
QUESTDB: a Database of Highly-Accurate Excitation Energies for the Electronic Structure Community
WIREs Comp. Mol. Sc. (IF=11.500), **11** (2021) e1517 (45 p) doi.
550. T. Pariat, P. M. V  rit  , D. Jacquemin*; J. Massue* and G. Ulrich*
2,2-Dipicolylamino Substituted 2-(2'-Hydroxybenzofuranyl) Benzoxazole (HBBO) Derivative : Towards Ratiometric Sensing of Divalent Zinc Cations
Dyes Pigm. (IF=5.122), **190** (2021) 109338 (6 p) doi.
551. J. Bosson*, G. M. Labrador, C. Besnard, D. Jacquemin* and J. Lacour*
Chiral Near-Infrared Fluorophores by Self-Promoted Oxidative Coupling of Cationic Helicenes with Amines/Enamines
Angew. Chem. Int. Ed. (IF=16.823), **60** (2021) 8733–8738 doi.
552. A. Kumar Gupta, W. Li, A. Ruseckas, C. Lian, C. L. Carpenter-Warren, D. B. Cordes, A. M. Z. Slawin, D. Jacquemin*, I. D. W. Samuel* and Eli Zysman-Colman*
Thermally Activated Delayed Fluorescence Emitters with Intramolecular Proton Transfer for High Luminance Solution-Processed Organic Light-Emitting Diodes
ACS Appl. Mat. Inter. (IF=10.383), **13** (2021) 15459–15474 doi.
553. R. J. Durand, S. Achelle, D. Robin-Le Guen, E. Caytan, N. Le Poul, A. Barsella, P. Guevara-Level, D. Jacquemin* and S. Gauthier*
Investigation of Second-Order Nonlinear Optical Responses in a Series of V-Shaped Binuclear Platinum (II) Complexes
Dalton Trans. (IF=4.569), **50** (2021) 4623–4633 doi.
554. J. D. Steen, D. R. Duijnste, A. S. Sardjan, J. Martinelli, L. Kortekaas, D. Jacquemin* and W. R. Browne*
Electrochemically Driven Ring Opening and Closing of a Spiropyran
J. Phys. Chem. A (IF=2.944), **125** (2021) 3355–3361 doi.
555. B. Osmialowski*, E. F. Petrusevich, K. C. Nawrot, B. K. Paszkiewicz, M. Nyk, J. Zielak, B. Jedrzejewska, J. M. Luis, D. Jacquemin* and R. Zalesny*
Tailoring Nonlinear Absorption of Fluorescent Dyes by Substitution at a Boron Center
J. Mater. Chem. C (IF=8.067), **9** (2021) 6225–6233 doi.
556. D. Jacquemin and J. P. Ceron-Carrasco*
Using Theory to Extend the Scope of Azobenzene Drugs in Chemotherapy: Novel Combinations for a Specific Delivery
ChemMedChem (IF=3.540), **16** (2021) 1764–1774 doi.
557. P. F. Loos*, D. A. Matthews F. Lipparini and D. Jacquemin*
How Accurate are EOM-CC4 Vertical Excitation Energies?
J. Chem. Phys. (IF=4.304), **154** (2021) 221103 (6 p) doi.
558. P. F. Loos*, M. Comin, X. Blase* and D. Jacquemin*
Reference Energies for Intramolecular Charge-Transfer Excitations
J. Chem. Theory Comput. (IF=6.578), **17** (2021) 3666–3686 doi.

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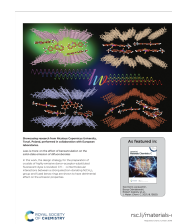
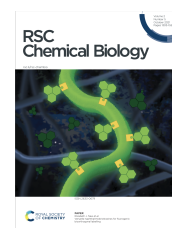
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Structure Illumination Microscopy Imaging of Lipid Vesicles in Live Bacteria with Naphthalimide-Appended Organometallic Complexes
Analyst (IF=5.227), **146** (2021) 3818–3822 doi.
560. Y. Yan, A. A. Sukhanov, M. H. E. Bousquet, Q. Guan, J. Zhao*, V. K. Voronkova*, D. Escudero*, Y. Xing*, G. G. Gurzadyan* and D. Jacquemin*
Does Twisted π -Conjugation Framework Always Induce Efficient Intersystem Crossing? A Case Study with Benzo[b]- and [a]phenanthrene-fused BODIPY Derivatives
J. Phys. Chem. B (IF=3.466), **125** (2021) 6280–6295 doi.
561. Z. Chen, S. Pascal, M. Daurat, L. Lichon, C. Nguyen, A. Godefroy, D. Durand, L. M. A. Ali, N. Bettache, Magali Gary-Bobo*, P. Arnoux, J. F. Longevial, A. D'Aléo, G. Marchand, D. Jacquemin* and O. Siri*
Modified Indulines: From Dyestuffs to in vivo Theranostic Agents
ACS Appl. Mat. Inter. (IF=10.383), **13** (2021) 30337–30349 doi.
562. M. Bondanza, D. Jacquemin and B. Mennucci*
Excited States of Xanthophylls Revised: Towards the Simulation of Biologically Relevant Systems
J. Phys. Chem. Lett. (IF=6.888), **12** (2021) 6604–6612 doi.
563. T. Stoerkler, D. Frath, D. Jacquemin*, J. Massue* and G. Ulrich*
Dual-State Emissive π -Extended Salicylaldehyde Fluorophores: Synthesis, Photophysical Properties and First-Principle Calculations
Eur. J. Org. Chem. (IF=3.261), (2021) 3726–3736 doi.
564. M. Pieczykolan, J. B. Derr*, A. Chrayteh, B. Koszarna, J. A. Clark, O. Vakuliuk, D. Jacquemin*, V. I. Vullev* and D. T. Gryko*
The Synthesis and Photophysical Properties of Weakly-Coupled Diketopyrrolopyrroles Molecules (IF=4.927), **26** (2021) 4744 (16p) doi.
565. C. A. Guido*, A. Chrayteh, G. Scalmani, B. Mennucci* and D. Jacquemin*
Simple Protocol for Capturing both Linear-Response and State-Specific Effects in Excited-State Calculations with Continuum Solvation Models
J. Chem. Theory Comput. (IF=6.578), **17** (2021) 5155–5164 doi.
566. I. C. D. Merritt, D. Jacquemin and M. Vacher*
Attochemistry: Is Controlling Electrons the Future of Photochemistry?
J. Phys. Chem. Lett. (IF=6.888), **12** (2021) 8404–8415 doi.
567. L. Breloy, Rana M., J. P. Malval, V. Brezova, D. Jacquemin*, S. Pascal, O. Siri* and D. L. Versace*
Azacalixphyryns as a Tremendous Alternative for the Free-Radical Photopolymerization under Visible and NIR Irradiation without the Need of Co-Initiators
Chem. Comm. (IF=6.065), **57** (2021) 8973–8976 doi.
568. K. Renault*, A. Chevalier, J. Bignon, D. Jacquemin*, J. A. Richard and A. Romieu*
Unprecedented Coumarin-Pyronin Hybrid Dyes: Synthesis, Fluorescence Properties and Theoretical Calculations
ChemPhotoChem (IF=3.679), **5** (2021) 822–838 doi.
569. I. C. D. Merritt, D. Jacquemin and M. Vacher*
Cis $\rightarrow$ Trans Photoisomerisation of Azobenzene: a Fresh Theoretical Look
Phys. Chem. Chem. Phys. (IF=3.945), **23** (2021) 19155–19165 doi.
570. E. Nikoloudakis, P. Baran Pati, G. Charalambidis, D. S. Budkina, D. Diring, A. Planchat, D. Jacquemin*, E. Vauthey*, A. G. Coutsolelos* and F. Odobel*
Dye-Sensitized PhotoElectrosynthesis Cell (DSPEC) for Benzyl Alcohol Oxidation using Zinc Porphyrin Sensitizer and TEMPO Catalyst
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578. P. F. Loos* and D. Jacquemin*
A Mountaineering Strategy to Excited States: Highly-Accurate Energies and Benchmarks for Bicyclic Systems
J. Phys. Chem. A (IF=2.944), **125** (2021) 10174–10188 [doi](#).
579. M. Tasior, P. Kowalczyk, M. Przybyl, M. Czichy, P. Janasik, M. H. E. Bousquet, M. Lapkowski*, M. Rammo, A. Rebane*, D. Jacquemin* and D. T. Gryko*
Going Beyond the Borders: Pyrrolo[3,2-b]pyrroles with Deep Red Emission
Chem. Sci. (IF=9.969), **12** (2021) 15935–15946 [doi](#).
580. T. Pariat, T. Stoerkler, C. Digu  t, A. D. Laurent*, D. Jacquemin*, J. Massue* and G. Ulrich*
Dual Solution/Solid-State Emissive Excited-State Intramolecular Proton Transfer (ESIPT) Dyes: a Combined Experimental and Theoretical Investigation
J. Org. Chem. (IF=4.198), **86** (2021) 17606–17619 [doi](#).
581. T. Delouche, G. Taifour, M. Cordier, T. Roisnel, D. Tondelier, P. Manzhi, B. Geffroy, B. Le Guennic, D. Jacquemin*, M. Hissler and P. A. Bouit*
Si-containing Polycyclic Aromatic Hydrocarbons: Synthesis and Opto-electronic Properties
Chem. Comm. (IF=4.9), **58** (2022) 88–91 [doi](#).
582. S. Aiken, G. K. Armitage, O. D. C. C. de Azevedo*, D. L. Crossley, R. Dobson*, C. D. Gabbutt, B. M. Heron*, D. Jacquemin*, C. R. Rice and N. Soltowska*
2,4,6-Tetraryl-2H-benzo[h]chromenes: the Influence of Electronic Communication between Aryl Substituents on their Photochromism
Dyes Pigm. (IF=4.5), **199** (2022) 110036 (24p) [doi](#).



583. S. Felder, M. L. Delcourt, M. H. E. Bousquet, D. Jacquemin*, R. Rodriguez, L. Favereau, J. Crassous*, L. Micouin* and E. Benedetti*
Planar Chiral Analogues of PRODAN Based on a [2.2]Paracyclophane Scaffold: Synthesis and Photophysical Studies
J. Org. Chem. (IF=3.6), **87** (2022) 147–158 doi.
584. K. V. Vygranenko, Y. M. Poronik, M. H. E. Bousquet, O. Vakuliuk, D. Jacquemin* and D. T. Gryko*
Direct Transformation of Coumarins into Orange-Red Emitting Rhodols: Unprecedented Reactivity of the Lactone Carbonyl Group
Chem. Comm. (IF=4.9), **58** (2022) 1542–1545 doi.
585. B. Salgues, R. Sarkar, M. L. Fajri, Y. A. Avalos-Quiros, A. D. Manick, M. Giorgi, N. Vanthuyne, Y. Carissan, C. Videt-Ackermann, J. Ackermann, G. Canard, J. L. Parrain, B. Le Guennic, D. Jacquemin*, M. Amatore, L. Commeiras, E. Zaborova* and F. Fages*
Synthesis and Electron Accepting Properties of Two Di(benz[f]indenone)-fused Tetraazaanthracene Isomers
J. Org. Chem. (IF=3.6), **87** (2022) 3276–3285 doi.
586. M. Munch, E. Colombain, T. Stoerkler, P. M. Vérité, D. Jacquemin*, J. Massue* and G. Ulrich*
Blue-Emitting 2-(2'-Hydroxyphenyl)Benzazole Fluorophores by Modulation of Excited-State Intramolecular Proton Transfer (ESIPT): Spectroscopic Studies and Theoretical Calculations
J. Phys. Chem. B (IF=3.3), **126** (2022) 2108–2118 doi.
587. H. J. Chang, M. V. Bondar, N. Munera, S. David, O. Maury, G. Berginc, B. Le Guennic, D. Jacquemin, C. Andraud, D. J. Hagan* and E. W. Van Stryland
Femtosecond Spectroscopy and Nonlinear Optical Properties of aza-BODIPY Derivatives in Solution
Chem. Eur. J. (IF=4.3), **28** (2022) e202104072 (8p) doi.
588. J. S. A. Badaro, B. Koszarna, M. H. E. Bousquet, E. T. Ouellette, D. Jacquemin* and D. T. Gryko*
The Kröhnke Synthesis of Benzo[a]indolizines Revisited: Towards Small, Red Light Emitters
Org. Chem. Front. (IF=5.4), **9** (2022) 1861–1874 doi.
589. G. D. Kumar, M. Banasiewicz, A. Wrzosek, R. Kempa, M. H. E. Bousquet, D. Jacquemin*, A. Szewczyk* and D. T. Gryko*
Probing Flux of Mitochondrial Potassium using an Azacrown-Diketopyrrolopyrrole based Highly Sensitive Probe
Chem. Comm. (IF=4.9), **58** (2022) 4500–4503 doi.
590. T. Stoerkler, T. Pariat, A. D. Laurent, D. Jacquemin*, G. Ulrich and J. Massue*
Excited-State Intramolecular Proton Transfer Dyes with Dual-State Emission Properties: Concept, Examples and Applications
Molecules (IF=4.6), **27** (2022) 2443 (17p) doi.
591. R. Sarkar, P. F. Loos, M. Boggio-Pasqua* and D. Jacquemin*
Assessing the Performances of CASPT2 and NEVPT2 for Vertical Excitation Energies
J. Chem. Theory Comput. (IF=5.5), **18** (2022) 2418–2436. doi.
592. F. Ceugniet, Q. Huauilmé, A. Sutter, D. Jacquemin*, N. Leclerc* and G. Ulrich*
Hetero-Substituted $\alpha\beta$ -Fused BODIPY
Chem. Eur. J. (IF=4.3), **28** (2022) e202200130 (9p) doi.
593. S. Budzak, J. Jovaisaite, C. Y. Huang, P. Baronas, K. Tulaite, S. Jursenas*, D. Jacquemin* and S. Hecht*
Mechanistic Insights into the Photoisomerization of N,N'-Disubstituted Indigos
Chem. Eur. J. (IF=4.3), **28** (2022) e202200496 (9p) doi.
594. M. Boggio-Pasqua*, D. Jacquemin* and P. F. Loos*
Benchmarking CASPT3 Vertical Excitation Energies
J. Chem. Phys. (IF=4.4), **157** (2022) 014103 (14p) doi.
595. P. F. Loos*, F. Lipparini, D. A. Matthews, A. Blondel and Denis Jacquemin*
A Mountaineering Strategy to Excited States: Revising Reference Values with EOM-CC4
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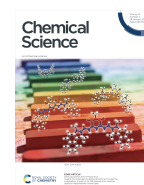
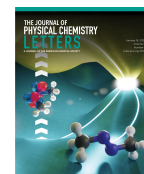
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Reference Energies for Cyclobutadiene: Automerization and Excited States
J. Phys. Chem. A (IF=2.9), **126** (2022) 4664–4679 [doi](#).
597. T. Delouche, E. Caytan, M. Cordier, T. Roisnel, G. Taupier, Y. Molard, N. Vanthuyne, B. Le Guennic, M. Hissler, D. Jacquemin* and P. A. Bouit*
Straightforward Access to Multifunctional π -Conjugated P-Heterocycles Featuring an Internal Ylidic Bond
Angew. Chem. Int. Ed. (IF=16.6), **61** (2022) e202205548 (9p) [doi](#).
598. K. S. Keremane, Y. Pellegrin, A. Planchat, P. Naik, D. Jacquemin*, F. Odobel* and A. V. Adhikari*
New Carbazole-based Dyads for p-Type DSSCs: Impact of Position of Acceptor Units on Device Performance
J. Phys. Chem. C (IF=3.7), **126** (2022) 12383–12390 [doi](#).
599. M. Durko-Maciag, D. Jacquemin*, G. Ulrich, J. Massue* and J. Mysliwiec*
Color-Tunable Multifunctional Excited-State Intramolecular Proton Transfer Emitter: Stimulated Emission of a Single Molecule
Chem. Eur. J. (IF=4.3), **28** (2022) e202201327 (9p) [doi](#).
600. M. Krzeszewski, S. Modrzycka, M. H. E. Bousquet, D. Jacquemin*, M. Drag* and D. T. Gryko*
Green-Emitting 4,5-Diaminonaphthalimides in Activity-based Probes for the Detection of Thrombin
Org. Lett. (IF=5.2), **24** (2022) 5602–5607 [doi](#).
601. T. Stoerkler, T. Pariat, A. D. Laurent, D. Jacquemin*, G. Ulrich*, and J. Massue*
Sterically Hindered 2-(2'-Hydroxyphenyl)benzoxazole (HBO) Emitters: Synthesis, Spectroscopic Studies, and Theoretical Calculations
Eur. J. Org. Chem. (IF=2.8), (2022) e202200661 (8p) [doi](#).
602. K. S. Keremane, Y. Pellegrin, D. Jacquemin*, F. Odobel* and A. V. Adhikari*
Push-pull Phenoxazine-based Sensitizers for p-Type DSSCs: Effect of Acceptor Units on Photovoltaic Performance
ChemSusChem (IF=8.4), **15** (2022) e202200520 (14p) [doi](#).
603. T. Baron, W. Naim, I. Nikolinakos, B. Andrin, Y. Pellegrin, D. Jacquemin*, S. Haacke*, F. Sauvage* and F. Odobel*
Transparent and Colorless Dye-Sensitized Solar Cells Based on Pyrrolopyrrole Cyanine Sensitizers
Angew. Chem. Int. Ed. (IF=16.6), **61** (2022) e202207459 (8p) [doi](#).
604. T. Horackova, M. H. E. Bousquet, A. Morice, U. Triballier, G. Canard, P. Lhotak, D. Jacquemin*, S. Pascal* and O. Siri*
Fully Zwitterionic Diaminobenzoquinonediimines Promoted by Cyanoaromatic N-substituents
Dyes Pigm. (IF=4.5), **206** (2022) 110681 (8p) [doi](#).
605. T. Castaing-Cordier, A. Benavides Restrepo, D. Dubois, V. Ladroue, F. Besacier, A. Buleté, C. Charvoz, A. Goupille, D. Jacquemin, P. Giraudeau and J. Farjon*
Characterization of New Psychoactive Substances by Integrating Benchtop NMR to Multi-technique Databases
Drug Test. Analysis (IF=2.9), **14** (2022) 1629–1638 [doi](#).
606. T. Olla, R. Jabbour, A. Labiod, O. Boyron, S. Méry, B. Heinrich, T. Heiser, D. Jacquemin, P. Lévêque, A. Lesage and N. Leclerc*
How Halogenation Impacts the Polymer Backbone Conformation: Learning from Combination of Solid-state MAS NMR and X-Ray Scattering
Adv. Func. Mater. (IF=19.0), **32** (2022) 202204929 (15p) [doi](#).
607. N. Ledos, T. Sangchai, I. Knysh, M. H. E. Bousquet, P. Manzhil, M. Cordier, D. Tondelier, B. Geffroy, D. Jacquemin*, P. A. Bouit* and M. Hissler*
Tuning the Charge Transfer in λ^5 -Phosphinines with Amino-Substituents
Org. Lett. (IF=5.2), **24** (2022) 6869–6873 [doi](#).

608. G. D. Kumar, M. Banasiewicz, A. Wrzosek, O. O'Mari, M. Zochowska, V. I. Vullev*, D. Jacquemin*, A. Szewczyk* and D. T. Gryko*
A Sensitive Diketopyrrolopyrrole-based Zinc Probe Operating via Enhancement of Excited-State Intramolecular Charge Transfer
Org. Biomol. Chem. (IF=3.2), **10** (2022) 7439–7447 [doi](#).
609. K. Ye, L. Cao, D. M. E. van Raamsdonk, Z. Wang, Z. Zhao*, D. Escudero* and D. Jacquemin*
Naphthalimide-Phenothiazine Dyads: Effect of Conformational Flexibility and Matching of the Energy of the Charge-Transfer State and the Localized Triplet Excited State on the Thermally Activated Delayed Fluorescence
Beilstein J. Org. Chem. (IF=2.7), **18** (2022) 1435–1453 [doi](#).
610. I. Knysh*, M. B. Jassar, B. Osmialowski, R. Zalesny* and D. Jacquemin*
In silico Screening of Two-photon Absorption Properties of a Large set of bis-BF₂-Dyes
ChemPhotoChem (IF=3.7), **6** (2022) e202200137 (9p) [doi](#).
611. T. Stoerkler, A. D. Laurent, G. Ulrich, D. Jacquemin* and J. Massue*
Influence of Ethynyl Extension on the Dual-State Emission Properties of Pyridinium-Substituted ESIPT Fluorophores
Dyes Pigm. (IF=4.5), **208** (2022) 110872 (8p) [doi](#).
612. I. Knysh, I. Duchemin, X. Blase* and D. Jacquemin*
Modelling Excited State Potential Energy Surfaces with Bethe-Salpeter Equation Formalism: The 4-(Dimethylamino)Benzonitrile Twist
J. Chem. Phys. (IF=4.4), **157** (2022) 194102 (13p) [doi](#).
613. P. Rybczyński, M. H. E. Bousquet, A. Kaczmarek-Kedziera, B. Jedrzejewska, D. Jacquemin* and B. Osmialowski*
Controlling the Fluorescence Quantum Yields of Benzothiazole-Difluoroborates by Optimal Substitution
Chem. Sci. (IF=8.4), **13** (2022) 13347–13360 [doi](#).
614. Xue Zhang, M. Ivanov, A. Wang, M. H. E. Bousquet, X. Liu, Y. Wan, J. Zhao*, A. Barbon*, D. Escudero*, D. Jacquemin* and M. Fedin*
Confinement of the Triplet States in π -Conjugated BODIPY Dimers Linked with Ethyne or Butadiyne Bridges: A Different View on the Effect of Symmetry
Angew. Chem. Int. Ed. (IF=16.6), **61** (2022) e202210419 (8p) [doi](#).
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Ground- and Excited-State Dipole Moments and Oscillator Strengths of Full Configuration Interaction Quality
J. Chem. Theory Comput. (IF=5.7), textbf19 (2023) 221–234 [doi](#).
616. M. Glodek, E. F. Petrushevich, D. Plazuk, D. Jacquemin* and B. Osmialowski*
Polyaromatic Hydrocarbon Antennas as Tools for Tuning properties of Push-Pull Difluoroborates
Dyes Pigm. (IF=4.1), **212** (2023) 111112 (8p) [doi](#).
617. C. Philippe, J. Melan, A. Barsella, T. Vibes, Y. R. Leroux, F. Robin-Le Guen, L. Lemiègre, D. Jacquemin*, S. Gauthier* and Y. Trolez*
A Comprehensive Study of Tetracyanobutadiene Push-Pull Chromophores Derived from γ -Pyranylidene Tetrahedron
Chem. (IF=NA), **5** (2023) 100036 (9p) [doi](#).
618. T. Stoerkler, P. Retailleau, D. Jacquemin, G. Ulrich and J. Massue*
Hetero-Aryl-Substituted bis-Anils: Aggregation-Induced Emission (AIE) Derivatives with Tunable ESIPT Emission Color and pH Sensitivity
Chem. Eur. J. (IF=3.9), **29** (2023) e202203766 (10p) [doi](#).
619. N. Ledos, D. Tondelier, B. Geffroy, D. Jacquemin*, P. A. Bouit* and M. Hissler*
Reaching the 5% Theoretical Limit of Fluorescent OLEDs with Push-Pull Benzophospholes
J. Mater. Chem. C (IF=5.7), **11** (2023) 3826–3831 [doi](#).

620. J. F. Longevial, I. Knysh, S. Al Shehim, L. Khrouz, A. Pandurangan, S. Pascal, G. Canard, C. Bucher*, D. Jacquemin* and O. Siri*
Proton-Coupled Electron Transfer in a Pivaloyl-Substituted Dihydro-Tetraazapentacene
Electrochim. Acta (IF=5.5), **449** (2023) 142224 (15p) [doi](#).
621. I. Knysh, K. Letellier, I. Duchemin, X. Blase* and D. Jacquemin*
Excited State Potential Energy Surfaces of N-Phenylpyrrole upon Twisting: Reference Values and Comparison Between BSE/GW and TD-DFT
Phys. Chem. Chem. Phys. (IF=2.9), **25** (2023) 8376–8385 [doi](#).
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Non-adiabatic Coupling in Trajectory Surface Hopping: How Approximations Impact Excited-State Reaction Dynamics
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Exploring Bethe-Salpeter Excited-State Dipoles: The Challenging Case of Increasingly Long Push-Pull Oligomers
J. Phys. Chem. Lett. (IF=4.8), **14** (2023) 3727–3734 [doi](#); Err: 5776–5776 [doi](#).
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Optical Signatures of Cisplatin Assembled with Curcuminoids: Theoretical Simulations to Develop Novel Anticancer Prodrugs
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625. E. F. Petrusevich, M. H. E. Bousquet, B. Ośmiałowski, D. Jacquemin*, J. M. Luis* and R. Zalesny*
Cost-Effective Simulations of Vibrationally-Resolved Absorption Spectra of Fluorophores with Machine-Learning-Based Inhomogeneous Broadening
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626. T. Munteanu, V. Mazan, M. Elhabiri, C. Benbouziyane, G. Canard, D. Jacquemin*, O. Siri* and S. Pascal*
A Strategy to Design Substituted Tetraamino-Phenazines and Access to a NIR-Absorbing Hexaamino-Phenazinium Dye
Org. Lett. (IF=4.9), **25** (2023) 3886–3891 [doi](#).
627. M. Durko-Maciag, G. Ulrich, D. Jacquemin, J. Mysliwiec* and J. Massue*
Solid-State Emitters Presenting a Modular Excited-State Proton Transfer (ESIPT) Process: Recent Advances in Dual-State Emission and Lasing Applications
Phys. Chem. Chem. Phys. (IF=2.9), **25** (2023) 15085–15098 [doi](#).
628. C. Figliola*, H. Anton, C. Sutter, P. Didier, D. Jacquemin* and G. Ulrich*
Lysosomes Targeting pH Activable Imaging-Guided Photodynamic Agents
ChemBioChem (IF=2.6), **24** (2023) e202300139 (10p) [doi](#).
629. T. Stoerkler, G. Ulrich, A. D. Laurent, D. Jacquemin* and J. Massue*
Interplay between Dual-State and Aggregation-Induced Emission with ESIPT Scaffolds Containing Triphenylamine Substituents: Experimental and Theoretical Studies
J. Org. Chem. (IF=3.3), **88** (2023) 9225–9236 [doi](#).
630. J. D. J. Villalobos-Castro, I. Knysh, D. Jacquemin, I. Duchemin and X. Blase*
Lagrangian Z-vector Approach to Bethe-Salpeter Analytic Gradients: Assessing Approximations
J. Chem. Phys. (IF=3.1), **159** (2023) 024116 (13p) [doi](#).
631. T. Sangchai, N. Ledos, A. Vacher, M. Cordier, B. Le Guennic, M. Hissler, D. Jacquemin* and P. A. Bouit*
Intrinsically Switchable Electroactive Fluorophores Based on λ^5 -Phosphinine Dimers
Chem. Eur. J. (IF=3.9), **29** (2023) e202301165 (9p) [doi](#).
632. T. Baron, W. Naim, I. Nikolinakos, B. Andrin, Y. Pellegrin, D. Jacquemin*, S. Haacke*, F. Sauvage* and F. Odobel*
Transparent and Colorless DSSC Featuring Thienyl-Pyrrolopyrrole Cyanine Sensitizers
J. Mater. Chem. A (IF=10.7), **11** (2023) 16767–16775 [doi](#).

633. F. Ceugniet*, A. Labiod, D. Jacquemin, B. Heinrich, F. Richard, P. L  v  que*, G. Ulrich and N. Leclerc*
Non-Fused BODIPY-Based Acceptor Molecules for Organic Photovoltaics
J. Mater. Chem. C (IF=5.7), **11** (2023) 10492–12501 [doi](#).
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Extensive Analysis of the Parameters Influencing Radiative Rates Obtained Through Vibronic Calculations
J. Chem. Theory Comput. (IF=5.7), **19** (2023) 5525–5547 [doi](#).
635. C. Maret, S. Chebourou, A. De Nicola, T. V. Papineau, M. Vacher, D. Jacquemin* and G. Ulrich*
Electron Rich Substituted β -Carboline Derivatives: Synthesis and Photophysical Properties
Dyes Pigm. (IF=4.1), **219** (2023) 111640 (8p) [doi](#).
636. T. Baron*, V. Maffei, C. Bucher, B. Le Guennic, A. Banyasz, D. Jacquemin*, G. Berginc*, O. Maury* and C. Andraud
Tuning the aza-BODIPYs Properties in the Near-Infrared with Thiophene Donor Substituents for Increasing the Charge Transfer
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Nonadiabatic Coupling in Trajectory Surface Hopping: Accurate Time Derivative Couplings by the Curvature-Driven Approximation
J. Chem. Theory Comput. (IF=5.7), **19** (2023) 6577–6588 (2023) [doi](#).
638. C. Elian, B. Mourot, C. Benbouziyane, J. P. Malval, S. Lajnef, F. Peyrot, O. Siri, D. Jacquemin*, S. Pascal* and D. L. Versace*
Tris-benzo[cd]indole Cyanine Enables the NIR-photosensitized Radical and Thiol-ene Polymerizations at 940 nm
Angew. Chem. Int. Ed. (IF=16.1), **62** (2023) e202305963 (9p) [doi](#).
639. I. Knysh, J. Villalobos-Castro, I. Duchemin, X. Blase* and D. Jacquemin*
Excess and Excited-State Dipole Moments of Real-Life Dyes: A Comparison Between Wave-Function, BSE/GW, and TD-DFT Values
Phys. Chem. Chem. Phys. (IF=2.9), **25** (2023) 29993–30004 [doi](#).
640. G. Sanil, M. Krzeszewski, W. Danikiewicz, L. Dobrzycki, I. Knysh, L. Dobrzycki, M. K. Cyrabski*, D. Jacquemin* and D. T. Gryko*
Unprecedented 1,2-Aryl Shift Accompanying Double Alkyne Benzannulation
Angew. Chem. Int. Ed. (IF=16.1), **62** (2023) e202311123 (9p) [doi](#).
Selected in Synfacts **20** (2024) 0055 [doi](#).
641. J. A. Clark, D. Kusy, O. Vakuliuk, M. Krzeszewski, K. J. Kochanowski, B. Koszarna, O. O'Mari, D. Jacquemin*, D. T. Gryko* and V. I. Vullev*
The Magic of Biaryl Linkages: Their Electronic Coupling through them Defines the Propensity for Excited-State Symmetry Breaking in Quadrupolar Acceptor-Donor-Acceptor Fluorophores
Chem. Sci. (IF=7.6), **14** (2023) 13537–13550 [doi](#).
642. P. F. Loos, F. Lipparini and D. Jacquemin*
Heptazine, Cyclazine, and Related Compounds: Chemically-Accurate Estimates of the Inverted Singlet-Triplet Gap
J. Phys. Chem. Lett. (IF=4.8), **14** (2023) 11069–11075 [doi](#); errata: **16** (2025) 2570–2570 [doi](#).
643. M. T. do Casal, K. Veys, Manon H. E. Bousquet, D. Escudero* and D. Jacquemin*
First-Principles Calculations of Excited-State Decay Rate Constants in Organic Fluorophores
J. Phys. Chem. A (IF=2.7), invited perspective, **127** (2023) 10033–10053 [doi](#).
644. D. Jacquemin*, F. Kossoski, F. Gam, M. Boggio-Pasqua* and P. F. Loos*
Reference Vertical Excitation Energies for Transition Metal Compounds
J. Chem. Theory Comput. (IF=5.7), **19** (2023) 8782–8800 [doi](#).

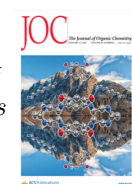
645. A. Chemin, I. Knysh, D. Ari, M. Cordier, T. Roisnel, B. Le Guennic, M. Hissler, D. Jacquemin* and P. A. Bouit*
Phospha-cyanines in their Ideal Polymethine State: Synthesis and Structure-Properties Relationships
J. Phys. Chem. A (IF=2.7), **127** (2023) 10457–10463 [doi](#).
646. K. Veys, M. H. E. Bousquet, D. Jacquemin and D. Escudero*
Modelling the Fluorescence Quantum Yields of Aromatic Compounds: Benchmarking the Machinery to Compute Intersystem Crossing Rates
J. Chem. Theory Comput. (IF=5.7), **19** (2023) 9344–9357 [doi](#).
647. J. Bosson*, M. Dirak, I. Knysh, D. Jacquemin* and S. Kolemen*
A Rapid Access to Activity-Based and Mitochondria Targeting Rhodol-Like Chromenoxanthene Dyes for Selective Bioimaging
Dyes Pigm. (IF=4.2) **223** (2024) 111952 (8p) [doi](#).
648. T. V. Papineau, D. Jacquemin and M. Vacher*
Non-Adiabatic Dynamics Simulations: Which Electronic Structure Method to Choose?
J. Phys. Chem. Lett. (IF=4.6), **15** (2024) 636–643 [doi](#).
649. B. Mourot, V. Mazan, M. Elhabiri, R. Sarkar, D. Jacquemin*, O. Siri and S. Pascal*
Insights into Extended Coupled Polymethines Through the Investigation of Dual UV-to-NIR Acidochromic Switches Based on Heptamethine-Oxonol Dyes
Chem. Sci. (IF=7.4), **15** (2024) 1248–1259 [doi](#).
650. P. Vazquez-Dominguez, J. F. Rizo, J. F. Arteaga, D. Jacquemin*, L. Favereau*, A. Ros* and U. Pischel*
Azaborahelicene Fluorophores Derived from Four-coordinate N,C-Boron Chelates: Synthesis, Photo-physical and Chiroptical Properties
Org. Chem. Front. (IF=4.7), **11** (2024) 843–853 [doi](#).
651. N. Ledos, D. Jacquemin*, P. A. Bouit* and M. Hissler*
Exploiting P-Chemistry to Modulate the Thermally Activated Delayed Fluorescence of Organic Fluorophores
Dyes Pigm. (IF=4.2), **224** (2024) 111978 (6p) [doi](#).
652. A. F. Henwood*, N. Curtin, S. Estalayo-Adrian, S. J. Aramballi, T. Gudmundsson, J. I. Lovitt, L. C. Sigurvinson, H. L. Dalton, C. S. Hawes, D. Jacquemin, D. F. O'Shea* and T. Gunnlaugsson*
Time-Resolved Fluorescence Imaging with Colour-Changing, “Turn-On/Turn-On” AIE Nanoparticles
Chem (IF=19.6), **10** (2024) 578–599 [doi](#).
653. C. Figliola*, A. Sutter, T. V. Papineau, C. Cheriaux, P. Retailleau, D. Jacquemin* and G. Ulrich*
Difluoro Dipyridomethene Boron Complexes: Synthesis, Characterization, and Ab Initio Calculations
J. Org. Chem. (IF=3.6), **89** (2024) 3020–3032 [doi](#).
654. F. Schnetz, I. Knysh, D. Jacquemin, S. Abbad Andaloussi, M. Presset, S. Lajnef, F. Peyrot and D. L. Versace*
Porphyrin-Based Photosensitizers for Visible-Light Polymerization and Antibacterial Applications
Polym. Chem. (IF=3.9), **15** (2024) 1377–1392 [doi](#).
655. M. Tasior, O. Vakuliuk, A. Wrzosek, V. I. Vullev*, A. Szewczyk*, D. Jacquemin* and D. T. Gryko*
Quadrupolar, Highly Polarized Dyes: Emission Dependence on Viscosity and Selective Mitochondria Staining
ACS Org. Inorg. Au (IF=4.4), **4** (2024) 248–257 [doi](#).
656. T. Castaing-Cordier, S. Crasnier, D. Dubois, V. Ladroue, A. Bulete, C. Prudhomme, C. Charvoz, F. Besacier, D. Jacquemin, P. Giraudeau* and Jonathan Farjon*
Non-Uniform Sampling to Enhance the Performance of Compact NMR for Characterizing New Psychoactive Substances
Magn. Reson. Chem. (IF=1.4), **95** (2024) 378–385 [doi](#).



657. I. Knysh, D. Rimbault, I. Duchemin, X. Blase* and D. Jacquemin*
Assessing the Accuracy of TD-DFT Excited-State Geometries through Optimal Tuning with GW Energy Levels
J. Chem. Phys. (IF=3.1), **160** (2024) 144115 (14p) [doi](#).
658. V. Delmas*, D. Jacquemin, A. Blondel, M. Vacher and A. D. Laurent*
How to Actively Learn Chemical Reactions Yields in Real-Time
React. Chem. Eng. (IF=3.1), **9** (2024) 1206–1215 [doi](#).
659. E. F. Petrushevich, H. Reis, B. Osmialowski, D. Jacquemin, J. M. Luis* and R. Zalesny*
One- and Two-Photon Absorption Spectra of Organoboron Complexes: Vibronic and Environmental Effects
Phys. Chem. Chem. Phys. (IF=2.9), **26** (2024) 13239–13250 [doi](#).
660. T. Stoerkler, G. Ulrich, P. Retailleau, A. D. Laurent, D. Jacquemin* and J. Massue*
Experimental and Theoretical Comprehension of ESIPT Fluorophores Based on a 2-(2'-Hydroxyphenyl)-3,3'-Dimethylindole (HDMI) Scaffold
Chem. Sci. (IF=7.4), **15** (2024) 7206–7218 [doi](#).
661. Y. Damour*, A. Scemama, D. Jacquemin, F. Kossoski* and P. F. Loos*
State-Specific Coupled-Cluster Methods for Excited States
J. Chem. Theory Comput. (IF=5.5), **20** (2024) 4129–4145 [doi](#).
662. T. Munteanu, J. F. Longevial, G. Canard, D. Jacquemin, S. Pascal* and O. Siri*
Post-Functionalization of Triamino-Phenaziniums Dyes to Reach Near-Infrared Emission
RSC Adv. (IF=4.6), **14** (2024) 19257–19263 [doi](#).
663. P. F. Loos and D. Jacquemin*
A Mountaineering Strategy to Excited States: Accurate Vertical Transition Energies and Benchmarks for Substituted Benzenes
J. Comput. Chem. (IF=4.8), **45** (2024) 1179–1805 [doi](#).
664. F. Kossoski*, M. Boggio-Pasqua*, P. F. Loos* and D. Jacquemin*
Reference Energies for Double Excitations: Improvement and Extension
J. Chem. Theory Comput. (IF=5.5), **20** (2024) 5655–5678 [doi](#).
665. T. Munteanu, D. Yordanov, G. Canard, O. Siri*, D. Jacquemin*, A. Georgiev* and S. Pascal*
Feasibility of Multiple Excited-State Proton Transfer Processes in Hydroxyquinoline-containing Benzoisimidazole Dyes
New J. Chem. (IF=2.5), **48** (2024) 13289–13295 [doi](#).
666. I. Knysh, F. Lipparini, A. Blondel, I. Duchemin, X. Blase, P. F. Loos* and D. Jacquemin*
Reference CC3 Excitation Energies for Organic Chromophores: Benchmarking TD-DFT, BSE/GW and Wave Function Methods
J. Chem. Theory Comput. (IF=5.5), **20** (2024) 8152–8174 [doi](#).
667. T. Stoerkler, A. Nicolas, J. El Aghar, G. Ulrich, A. D. Laurent, D. Jacquemin* and J. Massue*
Red-Shifting ESIPT Fluorescence by Site-Specific Functionalization in 2-(2'-Hydroxyphenyl)Benzazole Derivatives
ChemPhotoChem (IF=3.0), **8** (2024) e202400079 (11p) [doi](#).
668. T. Stoerkler, G. Ulrich, P. Retailleau, S. Achelle, A. D. Laurent, D. Jacquemin* and J. Massue*
Stimuli-Induced Fluorescence Switching in Azine-Containing Fluorophores Displaying Resonance-Stabilized ESIPT Fluorescence
Chem. Eur. J. (IF=3.7), **30** (2024) e02402448 (14p) [doi](#).
669. C. Naim*, R. Zalesny and D. Jacquemin*
Two-photon Absorption Strengths of Small Molecules: Reference CC3 Values and Benchmarks
J. Chem. Theory Comput. (IF=5.5), **20** (2024) 9093–9106 [doi](#).
670. P. Vázquez-Dominguez, M. Horojat, E. Suits, F. J. Fernández de Córdova, N. Vanthuyne, D. Jacquemin*, A. Ros* and L. Favereau*
Dual Luminescence and Infrared Circularly Polarized Luminescence up to 900 nm with Platinum

*Complexes Bearing Helical Donor-Acceptor Ligand*Mater. Chem. Front. (IF=6.4), **8** (2024) 3799–3806 doi.

671. G. Y. Erdemir, I. Knysh, K. Skonieczny, D. Jacquemin* and D. T. Gryko*
Tetracyanoethylene as a Building Block in the π -Expansion of 1,4-Dihydropyrrolo[3,2-b]pyrroles
J. Org. Chem. (IF=3.6), **89** (2024) 15513–15522 doi.
672. B. Salgues, R. Sarkar, N. Potier, A. D. Manick, G. Canard, J. L. Parrain, M. Giorgi, N. Vanthuyne, C. Videlot-Ackermann, J. Ackermann, F. Fages*, B. Le Guennic, D. Jacquemin, M. Amatore, E. Zaborova* and L. Commeiras*
Bis-Indeno-Fused Tetraazaanthracene Hybrids: Straightforward Synthesis and Studies of Optical and Electronic Properties
Eur. J. Org. Chem. (IF=2.7), **27** (2024) e202400719 (6p) doi.
673. B. Mourot, D. Jacquemin, O. Siri and S. Pascal*
Coupled Polymethines Dyes: Six Decades of Discoveries
Chem. Rec. (IF=7.5), **24** (2024) e202400183 (50p) doi.
674. Y. Aidibi, S. Azar, M. Voltz, L. Hardoin, M. Voltz, S. Goeb, M. Allain, M. Sallé, R. Costil, D. Jacquemin*, B. L. Feringa* and D. Canevet*
Light- and Temperature-Controlled Hybridization, Chiral Induction and Handedness of Helical Foldamers
Angew. Chem. Int. Ed. (IF=16.9), **64** (2025) e202413629 (8p) doi.
675. G. Sanil, L. Dobrzycki, M. K. Cyranski*, D. Jacquemin*, W. Chaladaj* and D. T. Gryko*
1,4-Dihydropyrrolo[3,2-b]pyrroles with Two Embedded Heptagons via Alkyne Annulation
J. Org. Chem. (IF=3.6), **90** (2025) 614–622 doi.
676. L. Ramirez Lazaro, L. C. Sigurvinsson, N. Curtin, J. Ho, E. T. Luis, D. McAdams, T. A. Gudmundsson, J. I. Lovitt, C. S. Hawes, D. Jacquemin, D. O'Shea, E. Scanlan, A. F. Henwood* and T. Gunnlaugsson*
Emissive Triphenylamine Functionalised 1,8-Naphthalimides and Naphthalene Diimide Fluorophores: Aggregation, Computation and Biological Studies
J. Mater. Chem. B (IF=5.7), **13** (2025) 929–942 doi.
677. V. Tarpa, J. F. Longevial, M. Giorgi, G. Canard, S. Pascal, D. Jacquemin* and O. Siri*
Transamination of Zwitterionic Quinones with Polyamines: The Carbon Bridge Matters
J. Org. Chem. (IF=3.6), **90** (2025) 1001–1005 doi.
678. L. Breloy, C. Elian, V. Alphonse, S. Lajnef, F. Peyrot, D. Jacquemin, S. Pascal, E. Devernois, T. Coradin, S. A. Andaloussi and D. L. Versace*
Terpenes, Natural Dyes and Photochemistry: Toward the Synthesis of Photoactive Bio-based Materials with Biocide Properties
RSC Appl. Polym. (IF=NA), **3** (2025) 222–237 doi.
679. B. Dupouy, L. Cotos, A. Binder, L. Slavikova, M. Rottmann, P. Mäser, D. Jacquemin, M. Ganter, E. Davioud-Charvet and M. Elhabiri*
Click Coupling of Flavylum Dyes with Plasmodione Analogues: Towards new Redox-Sensitive Profluorophores
Chem. Eur. J. (IF=3.7), **31** (2025) e202403691 (14p) doi.
680. K. Gorski, L. Pejov*, K. B. Jorgensen*, I. Knysh, D. Jacquemin* and D. T. Gryko*
Twofold 6π -Electrocyclization as a Route Toward Multi-heteroatom-doped Nanographenes Build on 1,4-Dihydropyrrolo[3,2-b]pyrrole Core
Chem. Eur. J. (IF=3.7), **31** (2025) e202404094 (10p) doi.
681. K. Gorski, S. Shelton, J. Lingagouder, P. Data*, D. Jacquemin* and D. T. Gryko*
1,4-Dihydropyrrolo[3,2-b]pyrrole Modified with Dibenzooxazepine: A Highly Efficient Core for Charge-Transfer-Based OLED Emitters
Chem. Sci. (IF=7.4), **16** (2025) 5223–5233 doi.



Hot Paper

⁴Starting from here, the 2024 IF are used.

682. T. Munteanu, C. Naim, G. Canard, D. Jacquemin*, O. Siri* and S. Pascal*
Small Far-Red Cationic Benzoquinone Diimine Dyes
Org. Biomol. Chem. (IF=2.7), **23** (2025) 2836–2844 [doi](#).
683. R. Sarkar, C. Naim, K. Ahmadzadeh, R. Zalesny*, D. Jacquemin* and J. M. Luis*
Simulations of Two-Photon Absorption Spectra of Fluorescent Dyes: The Impact of Non-Condon Effects
J. Chem. Theory Comput. (IF=5.5), **21** (2025) 3587–3599 [doi](#).
684. J. Sirucek, B. Le Guennic*, Y. Damour, P. F. Loos* and D. Jacquemin*
Excited State Absorption: Reference Oscillator Strengths, Wavefunction and TD-DFT Benchmarks
J. Chem. Theory Comput. (IF=5.5), **21** (2025) 4688–4703 [doi](#).
685. W. D. Petrykowski, N. Vanthuyne, C. Naim, F. Bertocchi, Y. M. Poronik, A. Ciesielski, M. K. Cyranski*, F. Terenziani*, D. Jacquemin* and D. T. Gryko*
Double Helicene Meets B-N Dative Bonds
Chem. Sci. (IF=7.4), **16** (2025) 8338–8345 [doi](#).
686. T. Stoerkler, D. Frath, G. Ulrich, P. Retailleau D. Jacquemin* and J. Massue*
Synthesis, Photophysical properties and ab initio Calculations of Dual Solution-Solid-State Emitting Ethynyl-Extended Boranil Complexes
J. Org. Chem. (IF=3.6), **90** (2025) 6980–6991 [doi](#).
687. C. Litot, M. Vansteelandt*, S. Ortiz, D. Barakat, E. Crossay, D. Tittton, S. Bourgeade-Delmas, C. Amasifuen, J. Graton, D. Jacquemin, J. L. Stigliani, M. Haddad and N. Fabre*
*New Cyclopeptides and γ -Butyrolactone Compounds from an Endophytic Strain of *Cophinforma Mamane**
ACS Omega (IF=4.3), **10** (2025) 21738–21746 [doi](#).
688. T. Stoerkler, T. Andris, G. Ulrich, A. D. Laurent D. Jacquemin* and J. Massue*
Impact of Aryl Extension on the Proton-Triggered Transition Switch in Azaheterocycle-Functionalized ESIPT Fluorophores
Dyes Pigm. (IF=4.2), **242** (2025) 112975 (8p) [doi](#).
689. T. Stoerkler, G. Ulrich, A. D. Laurent, D. Jacquemin* and J. Massue*
N-Aryl or N-Alkyl Pyridinium-Substituted ESIPT Fluorophores
ChemPlusChem (IF=2.8), **90** (2025) e202500138 (10p) [doi](#).
690. C. Chériaux, T. V. Papineau, P. Retailleau, C. Figliola*, D. Jacquemin* and G. Ulrich*
Insights into the Structure-Property Relationship of Difluoro Boron Dipyrromethene Derivatives
ChemPhotoChem (IF=3.0), **9** (2025) e202400395 (11p) [doi](#).
691. Y. Zhang, Z. Cui, J. Sirucek, D. Jacquemin*, B. Le Guennic*, X. Sun, X. D. Jiang* and G. Qin*
Embedding Oxygen Heterocycle into BODIPY to Enhance Intersystem Crossing for Photodynamic Therapy
J. Mater. Chem. B (IF=5.7), **13** (2025) 8833–8843 [doi](#).
692. P. F. Loos*, M. Boggio-Pasqua, A. Blondel, F. Lipparini and D. Jacquemin*
QUEST Database of Highly-Accurate Excitation Energies
J. Chem. Theory Comput. (IF=5.5), **21** (2025) 8010–8033 [doi](#).
693. S. Pascal*, A. Torres Ruiz, A. E. Baker, D. A. Vander Griend, M. Giorgi, A. Planchat, D. Jacquemin* and O. Siri*
Metastable Macrocyclic Bis-Meisenheimer
Angew. Chem. Int. Ed. (IF=16.9), **64** (2025) e202511037 (10p) [doi](#).
694. C. Naim* and D. Jacquemin*
Modeling the Emission Spectra and Radiative Decay Rates in Polychlorinated Organic Radicals
Phys. Chem. Chem. Phys. (IF=2.9), **27** (2025) 19970–19986 [doi](#).
695. B. Mourot, C. Naim, O. Siri, D. Jacquemin* and S. Pascal*
Synthesis and Properties of Quinoidal (Di-)Anionic Coupled Polymethine-Oxonol Dyes and Their Aromatic Counterparts
Org. Chem. Front. (IF=4.7), accepted [doi](#).



696. T. Stoerkler, G. Ulrich, A. D. Laurent, D. Jacquemin* and J. Massue*
Quinoline-Substituted Excited-State Intramolecular Proton Transfer Fluorophores as Stimuli-Sensitive Dual-State Fluorophores
Org. Chem. Front. (IF=4.7), accepted. [doi](#).
697. V. S. Yalissetty, S. Mandal, D. Jacquemin, T. Govindaraju* and P. Faller*
4-Dimethylamino-1,8-Naphthalimide as a Fluorescence Signal Amplification for Site Selective and Real Time Probing of the Hydroxyl Radical
Chem. Eur. J. (IF=3.7), **xxx** (2025) e02598 (10p) [doi](#).
698. C. Demangeat, M. Remond, J. M. Hudson, E. W. Evans, D. Jacquemin* and L. Favereau*
Symmetry Breaking and Hydrogen Bonding in Phthalimide compounds Enable Efficient Room-Temperature Circularly Polarized Phosphorescence in Solution
Angew. Chem. Int. Ed. (IF=16.9), **xxx** (2025) e202515218 (9p) [doi](#).
699. A. Rico, P. Le Poul, J. Rodriguez-Lopez, D. Jacquemin*, S. Achelle and S. Gauthier*
Multi-Stimuli-Responsive Chromic Properties of Soft Salts Based on Cyclometalated Platinum(II) Complexes: Pyridine- vs Pyrimidine-Based Ligands
ChemPhotoChem (IF=3.0), **xxx** (2025) e202500164 (9p) [doi](#).
700. K. Kikuchi, L. D. Adair, Y. Xu, H. J. Ross, Z. Lu, Y. Xiz, D. Jacquemin, R. P. Cox, T. D. M. Bell, N. L. Trevaskis, E. J. New and A. Kaur*
Exploring 4-Amino-1,8-Naphthalimides: Lifetime-based Sensing of Chemical Micro-environments
Chem. Eur. J. (IF=3.7), accepted.

B Chapters in books

1. D. Jacquemin*, E. A. Perpète, B. Champagne, J. M. André and B. Kirtman
Ab Initio Investigations of Polymethineimine Chains for Nonlinear Optics
in *Recent Research Developments in Physical Chemistry* (IF=NA), Research Signpost, G. Pandalai (Ed.)
Vol. **6** (2002) 145–165.
2. D. Y. Zhang*, C. Pouchan, D. Jacquemin and E. A. Perpète
Ab Initio Studies of Electronic First Hyperpolarizability of AB Systems Containing Phosphorus and Silicon Atoms
in *Lecture Series in Computer and Computational Sciences*, T. Simos, G. Maroulis (Ed.)
Adv. Comput. Methods Sci. Eng. (IF=NA), **4A–4B** (2005) 667–673.
3. D. Jacquemin*, E. A. Perpète and B. Kirtman
Calculation of Hartree-Fock Energy Derivatives in Polymers
in *Multiscale Modelling of Polymer Properties*, E. A. Perpète and M. Laso (Eds.), Computer-Aided Chemical Engineering Series (IF=NA), vol. 22
Chapter **1** (2006) 3–30 [isbn](#).
4. T. J. Shelton, B. Giner, C. S. Adjiman, A. Galindo, G. Jackson*, D. Jacquemin, V. Wathélet and E. A. Perpète
The Derivation of Size Parameters for the SAFT-VR Equation of State from Quantum Mechanical Calculation
in *Multiscale Modelling of Polymer Properties*, E. A. Perpète and M. Laso (Eds.), Computer-Aided Chemical Engineering Series (IF=NA), vol. 22
Chapter **7** (2006) 143–159 [isbn](#).
5. F. Odobel*, Y. Pellegrin, F. B. Anne and D. Jacquemin
Molecular Engineering of Efficient Dyes for P-type Semiconductor Sensitization
in *High-Efficiency Solar Cells: Physics, Materials and Devices*, X. Wang and Z. M. Wang (Eds.), Materials Science Series (IF=NA), vol. 190
Chapter **8** (2014) 215–246 [doi](#).
6. D. Jacquemin* and C. Adamo
Computational Molecular Electronic Spectroscopy with TD-DFT
in *Density-Functional Methods for Excited States*, N. Ferré, M. Filatov and M. Huix-Rotllant (Eds.)
Top. Curr. Chem. (IF=4.014), **368** (2016) 347–375 [doi](#).

7. D. E. Escudero*, A. D. Laurent* and D. Jacquemin*
Time-Dependent Density Functional Theory: A Tool to Explore Excited States
in *Handbook of Computational Chemistry*, J. Leszczynski (Ed.), 35 pp [doi](#).
8. M. Boggio-Pasqua, A. Perrier, A. Fihey and D. Jacquemin*
Modeling Diarylethenes Excited States with Ab initio Tools: from Model Systems to Large Multimers
in *Photon-Working Switches*, Y. Yokoyama and K. Nakatani (Eds.), Chap. 16 (2017) 321–341 [doi](#).

C Editorials

Most Accessed

1. M. E. Casida, H. Chermette and D. Jacquemin
Time-Dependent Density Functional Theory for Molecules and Molecular Solids
Editorial as guest editor of a special issue of J. Mol. Struct. (THEOCHEM)
J. Mol. Struct. (THEOCHEM) (IF=1.216), **914** (2009) 1–2 [doi](#).
2. D. Jacquemin*, L. Blancafort* and Y. M. Rhee*
Computational Photochemistry
Editorial as guest editor of a special issue of ChemPhotoChem
ChemPhotoChem (IF=2.838), **3** (2019) 664–665 [doi](#).
3. D. Jacquemin*, M. Wainwright*, and M. B. Heron*
Theory is Back in Dyes & Pigments!
Editorial of the journal promoting theory in this (mainly experimental) journal.
Dyes Pigm. (IF=4.889), **176** (2020) 108236 (1p) [doi](#).

D (Published) Proceedings

1. B. Champagne*, D. Jacquemin and J. M. André
Model Calculations of the First Hyperpolarizability per Unit Cell of Finite and Infinite Polymethineimine Chains
in *Nonlinear Optical Properties of Organic Materials VIII*, B. J. Thompson (Ed.)
Proc. SPIE (IF=0.077), **2527** (1995) 71–81 [doi](#).
2. D. Jacquemin*, B. Champagne and J. M. André
Asymmetric Unit Cell Polymers with Large First Hyperpolarizabilities
Synth. Met. (IF=1.376), **101** (1999) 490–491 [doi](#).
3. S. Pascal, A. Haefele, C. Monnereau, A. Charaf-Eddin, D. Jacquemin, B. Le Guennic, O. Maury* and C. Andraud*
On the Versatility of Electronic Structures in Polymethine Dyes
Proc. SPIE (IF=N/A), **9253** (2014) A (11p) [doi](#).
4. S. David*, D. Château, H. C. Chang, D. J. Hagan, E. W. Van Stryland, D. Jacquemin, C. Lopes, G. Berginc, S. Parola, O. Maury and C. Andraud
Aza-BODIPY Dyes for Optical Power Limitation in the SWIR: Molecular Engineering for Optimized Hybrid Materials
Proc. SPIE (IF=N/A), **11277** (2020) 25.
5. J. Bosson*, G. M. Labrador, D. Jacquemin* and J. Lacour*
Cationic [6]Helicenes: Tuning (Chir)Optical Properties up to the Near Infra-Red
Materials Today: Proceedings (IF= N/A), **62** (2022) 7751–7753 [doi](#).

E Popularization articles

1. D. Jacquemin*
Calcul Analytique du Module de Young des Polymères Stéréoréguliers
Chimie Nouvelle (IF=NA), **83** (2003) 124–124.
2. V. Wathélet, C. Michaux, M. Fontaine, J. M. André, D. Jacquemin and E. A. Perpète*
Paramétrisation d'Equations d'Etat sur Base de Descripteurs Moléculaires Estimés par la Mécanique Quantique
Techniques de l'Ingénieur (IF=NA), **AF6** (2008) n°052 (17 p.) [link](#).

3. A. D. Laurent*, V. Wathélet, M. Bouhy, D. Jacquemin and E. A. Perpète
Simulation de la Perception des Couleurs de Colorants Organiques
Techniques de l'Ingénieur (IF=NA), **AF6** (2010) n°810 (23 p.) [link](#).
4. J. P. Cerón-Carrasco*, D. Jacquemin, J. Zuniga and A. Requena
Claves Teóricas de la Mutación Espontánea en el ADN
An. Quím. (IF=N/A), **108** (2012) 197–204.
5. D. Jacquemin* and C. Daniel*
Molécules et Lumière : une Histoire d'Electrons
Actual. Chimique (IF=N/A), **382–383** (2014) 93–99.



F Patents

1. O. Siri, Z. Chen and D. Jacquemin
Analogues of Porphyrins, their Method of Preparation and Use Thereof
European Patent, EPO n° 12306044.4
2. K. Benelhadj, J. Massue, G. Ulrich, R. Ziessel, D. Jacquemin and A. D. Laurent
Emetteur Dual à Base d'Hydroxybenzazoles Substitués
European Patent, EP 2977374, WO 2016012457.
3. J. Rull-Barrull, M. d'Halluin, D. Jacquemin, E. Le Grogneec and F. X. Felpin
Méthode d'écriture réversible d'un motif sur un élément cellulosique et produit cellulosique associé
FR 16/00227
4. F. Odobel, F. Sauvage, D. Jacquemin, Y. Pellegrin, T. Baron, W. Naim
New Derivatives of Pyrrolopyrrole Cyanines and Uses Thereof
European Patent, EP 4019522.