

Denis Jacquemin: Publication list 1995–2025 (as 04/2025)

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 Polynes
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
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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](#).
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17. M. Spassova, T. Kolev, I. Kanev, D. Jacquemin and B. Champagne*
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J. Mol. Struct. (THEOCHEM) (IF=0.961), **528** (2000) 151–159 [doi](#).
18. E. A. Perpète*, B. Champagne and D. Jacquemin
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19. D. Jacquemin* and B. Champagne
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22. D. Jacquemin*, D. Beljonne, B. Champagne, V. Geskin, J. L. Brédas and J. M. André
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23. D. Jacquemin* and B. Champagne
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28. D. Jacquemin*, J. M. André and B. Champagne
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Pseudo Linear-Dependence and Long-Range Interaction on the Polarizability and Hyperpolarizabilities of Stereoregular Polymers
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33. D. Jacquemin*, C. Lambert and E. A. Perpète
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38. D. Jacquemin*, J. M. André and E. A. Perpète
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Int. J. Quantum Chem. (IF=1.192), **102** (2005) 209–223 [doi](#).
43. D. Jacquemin*
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47. D. Y. Zhang, C. Pouchan, D. Jacquemin* and E. A. Perpète
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50. D. Jacquemin*, J. Preat and E. A. Perpète
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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
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55. L. Briquet, D. P. Vercauteren, E. A. Perpète and D. Jacquemin*
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J. Chem. Theory Comput. (IF=3.627), **2** (2006) 434–440 [doi](#).
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65. J. Preat*, D. Jacquemin, V. Wathelet, J. M. André and E. A. Perpète
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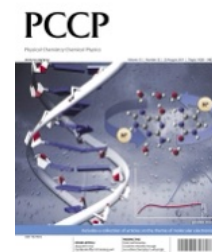
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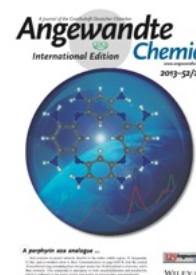


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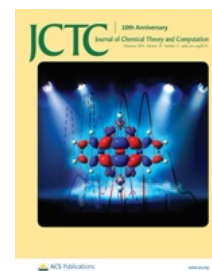
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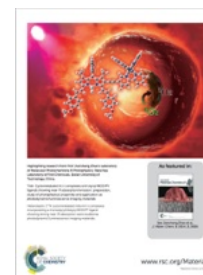
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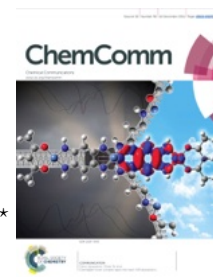
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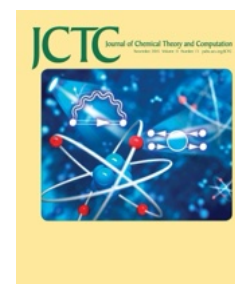
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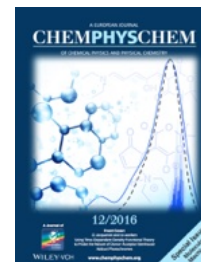
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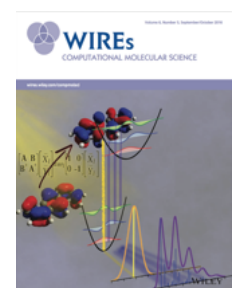
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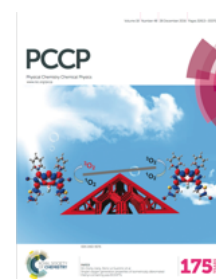
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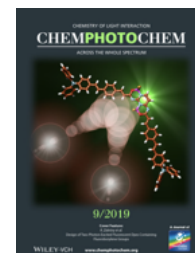
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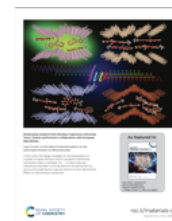
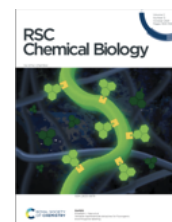
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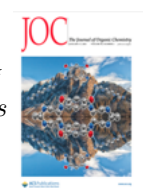
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