# Joseph G Fripiat

List of Publications by Year
in descending order



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|---|---|---|---|
| 40 papers | 527 citations | 840776 11 h-index | 677142 22 g-index |
| 41 all docs | 41 docs citations | 41 times ranked | 313 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Electronic Band Structure of Helical Polyisocyanides. Journal of Physical Chemistry A, 2017, 121, 7993-8002. | 2.5 | 1 |
| 2 | Fourier Space Uncoupled Hartreeâ€“Fock Polarizabilities of One-Dimensionally Periodic Systems. Polyethylene and Polysilane Revisited. Zeitschrift Fur Physikalische Chemie, 2016, 230, 589-632. | 2.8 | 1 |
| 3 | The Fourier Space Restricted Hartreeâ€“Fock Method for the Electronic Structure Calculation of One-Dimensionally Periodic Systems. Advances in Quantum Chemistry, 2015, 71, 153-194. | 0.8 | 0 |
| 4 | The Fourier space restricted Hartree-Fock method for the electronic structure calculation of linear poly(tetrafluoroethylene). Science China Chemistry, 2014, 57, 1355-1362. | 8.2 | 1 |
| 5 | Ewald-type formulas for Gaussian-basis studies of one-dimensionally periodic systems. Highlights in Theoretical Chemistry, 2014, , 181-187. | 0.0 | 0 |
| 6 | Ewald-type formulas for Gaussian-basis studies of one-dimensionally periodic systems. Theoretical Chemistry Accounts, 2012, 131, 1. | 1.4 | 5 |
| 7 | Ewald-type formulas for Gaussian-basis Bloch states in one-dimensionally periodic systems. Journal of Chemical Physics, 2010, 132, 044108. | 3.0 | 9 |
| 8 | Efficient calculation of the exchange in the Fourier representation of HFâ€LCAOâ€CO equations for 1D periodic systems. International Journal of Quantum Chemistry, 2009, 109, 2960-2967. | 2.0 | 5 |
| 9 | Fourier representation methods for MÃ¸llerâ€“Plesset perturbation theory in one-dimensionally periodic systems. Chemical Physics Letters, 2006, 422, 11-14. | 2.6 | 7 |
| 10 | Numerical integration of exchange energy in the two-dimensional Brillouin zone. Journal of Physics Condensed Matter, 2006, 18, 5493-5501. | 1.8 | 0 |
| 11 | Exchange contributions in the electronic structure of systems with 1D-periodicity: Importance and computation. International Journal of Quantum Chemistry, 2002, 90, 587-593. | 2.0 | 6 |
| 12 | Convergence of exchange lattice summations in direct-space polymer calculations. International Journal of Quantum Chemistry, 2002, 89, 452-463. | 2.0 | 9 |
| 13 | Virtues and potentialities of the Fourier transform method for electronic structure calculations of 1-D periodic systems at the Hartree-Fock level and beyond. International Journal of Quantum Chemistry, 2002, 90, 1326-1333. | 2.0 | 6 |
| 14 | MP2 correlation effects upon the electronic and vibrational properties of polyyne. Journal of Chemical Physics, 2001, 114, 5917-5922. | 3.0 | 26 |
| 15 | Computational aspects of polymer band structure calculations by the Fourier space restricted Hartree-Fock method. International Journal of Quantum Chemistry, 2000, 80, 856-862. | 2.0 | 11 |
| 16 | Unrestricted Hartreeâ€“Fock band structure calculations for polymers: Application to a cross-talk system. Journal of Chemical Physics, 2000, 113, 5958-5964. | 3.0 | 3 |
| 17 | Towards the Calculations of Polarizabilities of Stereoregular Polymers â™â™dedicated to Professor Yngve Ã–HRN at the occasion of his 65th birthday. Advances in Quantum Chemistry, 1999, , 95-110. | 0.8 | 7 |
| 18 | Dimerization versus complexation of triethylaluminum and diethylaluminum chloride: an ab initio determination of structures, energies of formation, and vibrational spectra. Computational and Theoretical Chemistry, 1998, 454, 149-159. | 1.5 | 11 |

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|---|---|---|---|
| 19 | Abinitioinvestigation of the electronic properties of planar and twisted polyparaphenylenes. Physical Review B, 1996, 54, 2381-2389. | 3.2 | 29 |
| 20 | On the convergence of the exchange-like sums in the random phase approximation applied to stereoregular polymers. International Journal of Quantum Chemistry, 1995, 56, 429-435. | 2.0 | 5 |
| 21 | Ab initio investigation of the static polarizability of planar and twisted infinite polythiophene chains. International Journal of Quantum Chemistry, 1994, 52, 451-467. | 2.0 | 18 |
| 22 | A Combined Analytical and Numerical Strategy to Solve the Atomic Hartree-Fock Equations in Momentum Space. Journal of Computational Physics, 1994, 111, 266-274. | 3.8 | 7 |
| 23 | Ab initio determination of polarizabilities per subunit in polymeric systems using the polarization propagator: Application to model hydrogen chains. International Journal of Quantum Chemistry, 1993, 46, 1-17. | 2.0 | 33 |
| 24 | Efficient computation of electron-repulsion integrals inab initio studies of polymeric systems. International Journal of Quantum Chemistry, 1993, 48, 793-806. | 2.0 | 9 |
| 25 | <title>Ab initio Hartree Fock longitudinal polarizabilities per subunit of stereoregular polymers</title>. , 1993, 1775, 236. | | 2 |
| 26 | From uncoupled to coupled Hartreeâ€“Fock polarizabilities of infinite polymeric chains. Pariserâ€“Parrâ€“Pople applications to the polyacetylene chains. Journal of Chemical Physics, 1992, 96, 8330-8337. | 3.0 | 51 |
| 27 | Improving the one-electron states of ab initio LCAO-GTO calculations in momentum space. Application to Be and B+ atoms. Computational and Theoretical Chemistry, 1992, 254, 145-159. | 1.5 | 11 |
| 28 | Structural and electronic analysis of peripheral benzodiazepine ligands: Description of the pharmacophoric elements for their receptors. International Journal of Quantum Chemistry, 1990, 38, 1-25. | 2.0 | 11 |
| 29 | Delocalization of the acid function in molecular sieves. Zeolites, 1990, 10, 221-222. | 0.5 | 8 |
| 30 | Improving the Oneâ€Electron States of ab initio GTO Calculations in Momentum Space. Tests on twoâ€Electron Systems: H<sup>â^'</sup>, He and Li<sup>â^'+</sup>. Bulletin Des SociÃ©tÃ©s Chimiques Belges, 1990, 99, 135-145. | 0.0 | 6 |
| 31 | On the restricted Hartree-Fock description of oligomer chains with expected metallic character. Computational and Theoretical Chemistry, 1988, 179, 393-406. | 1.5 | 3 |
| 32 | Gas-phase ultraviolet photoelectron spectroscopic study of the 3,7-diphenyl- and 3,7-bis(dimethylamino)-1,5-dithia-2,4,6,8-tetrazocines. Journal of the Chemical Society Perkin Transactions II, 1987, , 259. | 0.9 | 3 |
| 33 | Equilbrium geometry and electrical polarizability of formic acid, formamide and their cyclic hydrogen-bonded paris. International Journal of Quantum Chemistry, 1987, 32, 85-103. | 2.0 | 13 |
| 34 | Structure Ã©lectronique des dianions B12H122â^' et B9C2Hn2â^'. Canadian Journal of Chemistry, 1986, 64, 1752-1757. | 1.1 | 13 |
| 35 | Electron density and related properties in stereoregular polymers and biopolymers. Journal of Computational Chemistry, 1984, 5, 349-352. | 3.3 | 3 |
| 36 | Evaluation of computational aspects of a modified CS-LCAO-SCF-CO strategy for electronic structure calculations of extended model chains. International Journal of Quantum Chemistry, 1984, 26, 141-152. | 2.0 | 17 |

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|---|---|---|---|
| 37 | Non-empirical quantum mechanical calculations on pentasil-type zeolites. Zeolites, 1983, 3, 306-310. | 0.5 | 91 |
| 38 | On the behaviour of exchange in restricted hartree-fock-roothaan calculations for periodic polymers. Chemical Physics Letters, 1981, 77, 143-150. | 2.6 | 50 |
| 39 | On the use of laplace transform to evaluate one-dimensional lattice summations in quantum calculations of model polymers. International Journal of Quantum Chemistry, 1980, 18, 431-442. | 2.0 | 1 |
| 40 | Quantum mechanical approach to the chemisorption of molecular hydrogen on defect magnesium oxide surfaces. Theoretica Chimica Acta, 1977, 43, 239-251. | 0.8 | 30 |