Joseph G Fripiat

List of Publications by Year
in descending order

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

840776

677142

#	Article	IF	Citations
1	Non-empirical quantum mechanical calculations on pentasil-type zeolites. Zeolites, 1983, 3, 306-310.	0.5	91
2	From uncoupled to coupled Hartree–Fock polarizabilities of infinite polymeric chains. Pariser–Parr–Pople applications to the polyacetylene chains. Journal of Chemical Physics, 1992, 96, 8330-8337.	3.0	51
3	On the behaviour of exchange in restricted hartree-fock-roothaan calculations for periodic polymers. Chemical Physics Letters, 1981, 77, 143-150.	2.6	50
4	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
5	Quantum mechanical approach to the chemisorption of molecular hydrogen on defect magnesium oxide surfaces. Theoretica Chimica Acta, 1977, 43, 239-251.	0.8	30
6	Abinitioinvestigation of the electronic properties of planar and twisted polyparaphenylenes. Physical Review B, 1996, 54, 2381-2389.	3.2	29
7	MP2 correlation effects upon the electronic and vibrational properties of polyyne. Journal of Chemical Physics, 2001, 114, 5917-5922.	3.0	26
8	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
9	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
10	Structure électronique des dianions B12H122⁻ et B9C2Hn2⁻. Canadian Journal of Chemistry, 1986, 64, 1752-1757.	1.1	13
11	Equilbrium geometry and electrical polarizability of formic acid, formamide and their cyclic hydrogen-bonded pairs. International Journal of Quantum Chemistry, 1987, 32, 85-103.	2.0	13
12	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
13	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
14	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
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	Efficient computation of electron-repulsion integrals inab initio studies of polymeric systems. International Journal of Quantum Chemistry, 1993, 48, 793-806.	2.0	9
17	Convergence of exchange lattice summations in direct-space polymer calculations. International Journal of Quantum Chemistry, 2002, 89, 452-463.	2.0	9
18	Ewald-type formulas for Gaussian-basis Bloch states in one-dimensionally periodic systems. Journal of Chemical Physics, 2010, 132, 044108.	3.0	9

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19	Delocalization of the acid function in molecular sieves. Zeolites, 1990, 10, 221-222.	0.5	8
20	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
21	Towards the Calculations of Polarizabilities of Stereoregular Polymers ™â™dedicated to Professor Yngve Ã—HRN at the occasion of his 65th birthday. Advances in Quantum Chemistry, 1999, , 95-110.	0.8	7
22	Fourier representation methods for MÃ¸llerâ€"Plesset perturbation theory in one-dimensionally periodic systems. Chemical Physics Letters, 2006, 422, 11-14.	2.6	7
23	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
24	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
25	Improving the Oneâ€Electron States of <i>ab initio</i> GTO Calculations in Momentum Space. Tests on twoâ€Electron Systems: H^{â˜'}, He and Li^{â˜'+}. Bulletin Des SociÃ©tÃ©s Chimiques Belges, 1990, 99, 135-145.	0.0	6
26	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
27	Efficient calculation of the exchange in the Fourier representation of HFâ€ŁCAOâ€€O equations for 1D periodic systems. International Journal of Quantum Chemistry, 2009, 109, 2960-2967.	2.0	5
28	Ewald-type formulas for Gaussian-basis studies of one-dimensionally periodic systems. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	5
29	Electron density and related properties in stereoregular polymers and biopolymers. Journal of Computational Chemistry, 1984, 5, 349-352.	3.3	3
30	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
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	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
33	<title>Ab initio Hartree Fock longitudinal polarizabilities per subunit of stereoregular polymers</title>. , 1993, 1775, 236.		2
34	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
35	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
36	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

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37	Electronic Band Structure of Helical Polyisocyanides. Journal of Physical Chemistry A, 2017, 121, 7993-8002.	2.5	1
38	Numerical integration of exchange energy in the two-dimensional Brillouin zone. Journal of Physics Condensed Matter, 2006, 18, 5493-5501.	1.8	0
39	The Fourier Space Restricted Hartree–Fock Method for the Electronic Structure Calculation of One-Dimensionally Periodic Systems. Advances in Quantum Chemistry, 2015, 71, 153-194.	0.8	0
40	Ewald-type formulas for Gaussian-basis studies of one-dimensionally periodic systems. Highlights in Theoretical Chemistry, 2014, , 181-187.	0.0	0