Michel Dupuis

List of Publications by Year
in descending order

53	6,309	136740 32	168136 53
papers	citations	h-index	g-index

53	53	53	6506
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Evaluation of molecular integrals over Gaussian basis functions. Journal of Chemical Physics, 1976, 65, 111-116.	1.2	718
2	High performance computational chemistry: An overview of NWChem a distributed parallel application. Computer Physics Communications, 2000, 128, 260-283.	3.0	698
3	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	1.2	425
4	Electron transport via polaron hopping in bulkTiO2: A density functional theory characterization. Physical Review B, 2007, 75, .	1.1	394
5	Electric-field induced intramolecular electron transfer in spiro .pi.-electron systems and their suitability as molecular electronic devices. A theoretical study. Journal of the American Chemical Society, 1990, 112, 4206-4214.	6.6	348
6	Charge transport in metal oxides: A theoretical study of hematite Î±-Fe2O3. Journal of Chemical Physics, 2005, 122, 144305.	1.2	281
7	An ab initio model of electron transport in hematite (Î±-Fe2O3) basal planes. Journal of Chemical Physics, 2003, 118, 6455-6466.	1.2	274
8	Water oxidation on a mononuclear manganese heterogeneous catalyst. Nature Catalysis, 2018, 1, 870-877.	16.1	244
9	Distribution of Ti³⁺ Surface Sites in Reduced TiO₂. Journal of Physical Chemistry C, 2011, 115, 7562-7572.	1.5	235
10	Molecular symmetry. II. Gradient of electronic energy with respect to nuclear coordinates. Journal of Chemical Physics, 1978, 68, 3998-4004.	1.2	230
11	Computation of electron repulsion integrals using the rys quadrature method. Journal of Computational Chemistry, 1983, 4, 154-157.	1.5	209
12	Defining the Role of Excess Electrons in the Surface Chemistry of TiO₂. Journal of Physical Chemistry C, 2010, 114, 5891-5897.	1.5	202
13	Localized Electronic States from Surface Hydroxyls and Polarons in TiO₂(110). Journal of Physical Chemistry C, 2009, 113, 14583-14586.	1.5	196
14	Intrinsic Hole Migration Rates in TiO₂from Density Functional Theory. Journal of Physical Chemistry C, 2009, 113, 346-358.	1.5	166
15	Molecular symmetry and closed-shellSCF calculations. I. International Journal of Quantum Chemistry, 1977, 11, 613-625.	1.0	165
16	Efficient hydrogen peroxide synthesis by metal-free polyterthiophene via photoelectrocatalytic dioxygen reduction. Energy and Environmental Science, 2020, 13, 238-245.	15.6	146
17	Interfacial Charge Modulation: An Efficient Strategy for Boosting Spatial Charge Separation on Semiconductor Photocatalysts. Advanced Energy Materials, 2019, 9, 1803951.	10.2	125
18	The nature of photogenerated charge separation among different crystal facets of BiVO₄studied by density functional theory. Physical Chemistry Chemical Physics, 2015, 17, 23503-23510.	1.3	112

#	Article	IF	Citations
19	On the determination of the minimum on the crossing seam of two potential energy surfaces. Journal of Computational Chemistry, 1991, 12, 276-282.	1.5	98
20	The general atomic and molecular electronic structure system hondo: Version 7.0. Computer Physics Communications, 1989, 52, 415-425.	3.0	79
21	Structure, vibrational spectra, and IR intensities of polyenes from ab initio SCF calculations. Journal of Chemical Physics, 1988, 88, 1003-1009.	1.2	71
22	Hybrid approach for free energy calculations with high-level methods: Application to the SN2 reaction of CHCl3 and OHâ^' in water. Journal of Chemical Physics, 2007, 127, 051102.	1.2	70
23	Electron transfer in environmental systems: a frontier for theoretical chemistry. Theoretical Chemistry Accounts, 2006, 116, 124-136.	0.5	59
24	Molecular symmetry. III. Second derivatives of electronic energy with respect to nuclear coordinates. Journal of Chemical Physics, 1981, 75, 332-336.	1.2	54
25	Theoretical prediction of the vibrational spectrum of naphthalene in the first excited singlet state. Journal of Chemical Physics, 1993, 98, 974-987.	1.2	52
26	Charge carrier transport dynamics in W/Mo-doped BiVO₄: first principles-based mesoscale characterization. Journal of Materials Chemistry A, 2019, 7, 3054-3065.	5.2	51
27	Theoretical and experimental studies of optical nonlinearities of haloforms CHX3, X=F, Cl, Br, I. Journal of Chemical Physics, 1990, 92, 7418-7425.	1.2	49
28	Reorganization energy associated with small polaron mobility in iron oxide. Journal of Chemical Physics, 2004, 120, 7050-7054.	1.2	46
29	Role of Oxygen Vacancies on Oxygen Evolution Reaction Activity: Î²-Ga₂O₃ as a Case Study. Chemistry of Materials, 2018, 30, 7714-7726.	3.2	43
30	Abinitioselfâ€consistentâ€field molecular orbital calculations on defects associated with radiation damage in alpha quartz. Journal of Chemical Physics, 1991, 95, 4215-4224.	1.2	38
31	Combined Quantum Mechanical and Molecular Mechanics Studies of the Electron-Transfer Reactions Involving Carbon Tetrachloride in Solution. Journal of Physical Chemistry A, 2008, 112, 2713-2720.	1.1	36
32	Amorphous Cobalt Oxide Nanoparticles as Active Waterâ€Oxidation Catalysts. ChemCatChem, 2017, 9, 3641-3645.	1.8	34
33	Water Oxidation on Oxygen-Deficient Barium Titanate: A First-Principles Study. Journal of Physical Chemistry C, 2017, 121, 8378-8389.	1.5	34
34	Ab initio SCF molecular dynamics: Exploring the potential energy surface of small silicon clusters. International Journal of Quantum Chemistry, 1992, 42, 1327-1338.	1.0	32
35	Water Oxidation on TiO₂: A Comparative DFT Study of 1e^{â€“}, 2e^{â€“}, and 4e^{â€“} Processes on Rutile, Anatase, and Brookite. Journal of Physical Chemistry C, 2020, 124, 8094-8100.	1.5	30
36	Parallel computation of the MP2 energy on distributed memory computers. Journal of Computational Chemistry, 1995, 16, 395-404.	1.5	29

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37	Defects in doped polyacetylene: An ab initio infrared and Raman spectroscopy of solitons. Journal of Chemical Physics, 1988, 88, 5252-5254.	1.2	26
38	New integral transforms for molecular properties and application to a massively parallel GIAO-SCF implementation. Computer Physics Communications, 2001, 134, 150-166.	3.0	26
39	Band Structure Engineering: Insights from Defects, Band Gap, and Electron Mobility, from Study of Magnesium Tantalate. Journal of Physical Chemistry C, 2016, 120, 6930-6937.	1.5	26
40	Unravelling the water oxidation mechanism on NaTaO₃-based photocatalysts. Journal of Materials Chemistry A, 2020, 8, 6812-6821.	5.2	23
41	Bimodal hole transport in bulk BiVO₄ from computation. Journal of Materials Chemistry A, 2018, 6, 3714-3723.	5.2	20
42	Hole Polaron Transport in Bismuth Vanadate BiVO₄ from Hybrid Density Functional Theory. Journal of Physical Chemistry C, 2020, 124, 23038-23044.	1.5	20
43	Photocatalytic Facet Selectivity in BiVO4 Nanoparticles: Polaron Electronic Structure and Thermodynamic Stability Considerations for Photocatalysis. Journal of Physical Chemistry C, 2019, 123, 20142-20151.	1.5	18
44	Ethylene and Water Co-Adsorption on Ag/SSZ-13 Zeolites: A Theoretical Study. Journal of Physical Chemistry C, 2020, 124, 7295-7306.	1.5	18
45	Defects in doped polyacetylene: An ab initio infrared and Raman spectroscopy of solitons. Journal of Chemical Physics, 1988, 88, 2859-2860.	1.2	15
46	Electron transfer in extended systems: characterization by periodic density functional theory including the electronic coupling. Physical Chemistry Chemical Physics, 2020, 22, 10609-10623.	1.3	11
47	Synthesis and Anisotropic Electrocatalytic Activity of Covellite Nanoplatelets with Fixed Thickness and Tunable Diameter. ACS Applied Materials & Interfaces, 2018, 10, 42417-42426.	4.0	10
48	Ab initio Hartreeâ€“Fock energy band structure calculations on polyaniline. Journal of Chemical Physics, 1987, 86, 6309-6313.	1.2	9
49	Integral data compression for FPS 64-BIT processors: Improved I/O and reduced storage. Journal of Computational Chemistry, 1988, 9, 148-157.	1.5	5
50	Quantum Mechanical Simulations of Polymers for Molecular Electronics and Photonics. ACS Symposium Series, 1987, , 146-161.	0.5	3
51	Maximal orbital analysis of molecular wavefunctions. Journal of Computational Chemistry, 2019, 40, 39-50.	1.5	3
52	Charge Carrier Management in Semiconductors: Modeling Charge Transport and Recombination. Springer Handbooks, 2022, , 365-398.	0.3	2
53	Ab Initio Self-Consistent Field-Molecular Orbital Calculations Including Long-Range Coulomb Effects. ACS Symposium Series, 1987, , 69-80.	0.5	1