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	Charge Carrier Management in Semiconductors: Modeling Charge Transport and Recombination. Springer Handbooks, 2022, , 365-398.	0.3	2
2	Efficient hydrogen peroxide synthesis by metal-free polyterthiophene via photoelectrocatalytic dioxygen reduction. Energy and Environmental Science, 2020, 13, 238-245.	15.6	146
3	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
4	Hole Polaron Transport in Bismuth Vanadate BiVO₄ from Hybrid Density Functional Theory. Journal of Physical Chemistry C, 2020, 124, 23038-23044.	1.5	20
5	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	1.2	425
6	Unravelling the water oxidation mechanism on NaTaO₃-based photocatalysts. Journal of Materials Chemistry A, 2020, 8, 6812-6821.	5.2	23
7	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
8	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
9	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
10	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
11	Interfacial Charge Modulation: An Efficient Strategy for Boosting Spatial Charge Separation on Semiconductor Photocatalysts. Advanced Energy Materials, 2019, 9, 1803951.	10.2	125
12	Maximal orbital analysis of molecular wavefunctions. Journal of Computational Chemistry, 2019, 40, 39-50.	1.5	3
13	Bimodal hole transport in bulk BiVO₄ from computation. Journal of Materials Chemistry A, 2018, 6, 3714-3723.	5.2	20
14	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
15	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
16	Water oxidation on a mononuclear manganese heterogeneous catalyst. Nature Catalysis, 2018, 1, 870-877.	16.1	244
17	Amorphous Cobalt Oxide Nanoparticles as Active Waterâ€Oxidation Catalysts. ChemCatChem, 2017, 9, 3641-3645.	1.8	34
18	Water Oxidation on Oxygen-Deficient Barium Titanate: A First-Principles Study. Journal of Physical Chemistry C, 2017, 121, 8378-8389.	1.5	34

#	Article	IF	Citations
19	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
20	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
21	Distribution of Ti³⁺ Surface Sites in Reduced TiO₂. Journal of Physical Chemistry C, 2011, 115, 7562-7572.	1.5	235
22	Defining the Role of Excess Electrons in the Surface Chemistry of TiO₂. Journal of Physical Chemistry C, 2010, 114, 5891-5897.	1.5	202
23	Localized Electronic States from Surface Hydroxyls and Polarons in TiO₂(110). Journal of Physical Chemistry C, 2009, 113, 14583-14586.	1.5	196
24	Intrinsic Hole Migration Rates in TiO₂from Density Functional Theory. Journal of Physical Chemistry C, 2009, 113, 346-358.	1.5	166
25	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
26	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
27	Electron transport via polaron hopping in bulkTiO2: A density functional theory characterization. Physical Review B, 2007, 75, .	1.1	394
28	Electron transfer in environmental systems: a frontier for theoretical chemistry. Theoretical Chemistry Accounts, 2006, 116, 124-136.	0.5	59
29	Charge transport in metal oxides: A theoretical study of hematite Î±-Fe2O3. Journal of Chemical Physics, 2005, 122, 144305.	1.2	281
30	Reorganization energy associated with small polaron mobility in iron oxide. Journal of Chemical Physics, 2004, 120, 7050-7054.	1.2	46
31	An ab initio model of electron transport in hematite (Î±-Fe2O3) basal planes. Journal of Chemical Physics, 2003, 118, 6455-6466.	1.2	274
32	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
33	High performance computational chemistry: An overview of NWChem a distributed parallel application. Computer Physics Communications, 2000, 128, 260-283.	3.0	698
34	Parallel computation of the MP2 energy on distributed memory computers. Journal of Computational Chemistry, 1995, 16, 395-404.	1.5	29
35	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
36	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

#	Article	IF	Citations
37	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
38	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
39	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
40	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
41	The general atomic and molecular electronic structure system hondo: Version 7.0. Computer Physics Communications, 1989, 52, 415-425.	3.0	79
42	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
43	Defects in doped polyacetylene: An ab initio infrared and Raman spectroscopy of solitons. Journal of Chemical Physics, 1988, 88, 5252-5254.	1.2	26
44	Defects in doped polyacetylene: An ab initio infrared and Raman spectroscopy of solitons. Journal of Chemical Physics, 1988, 88, 2859-2860.	1.2	15
45	Structure, vibrational spectra, and IR intensities of polyenes from ab initio SCF calculations. Journal of Chemical Physics, 1988, 88, 1003-1009.	1.2	71
46	Quantum Mechanical Simulations of Polymers for Molecular Electronics and Photonics. ACS Symposium Series, 1987, , 146-161.	0.5	3
47	Ab initio Hartreeâ€“Fock energy band structure calculations on polyaniline. Journal of Chemical Physics, 1987, 86, 6309-6313.	1.2	9
48	Ab Initio Self-Consistent Field-Molecular Orbital Calculations Including Long-Range Coulomb Effects. ACS Symposium Series, 1987, , 69-80.	0.5	1
49	Computation of electron repulsion integrals using the rys quadrature method. Journal of Computational Chemistry, 1983, 4, 154-157.	1.5	209
50	Molecular symmetry. III. Second derivatives of electronic energy with respect to nuclear coordinates. Journal of Chemical Physics, 1981, 75, 332-336.	1.2	54
51	Molecular symmetry. II. Gradient of electronic energy with respect to nuclear coordinates. Journal of Chemical Physics, 1978, 68, 3998-4004.	1.2	230
52	Molecular symmetry and closed-shellSCF calculations. I. International Journal of Quantum Chemistry, 1977, 11, 613-625.	1.0	165
53	Evaluation of molecular integrals over Gaussian basis functions. Journal of Chemical Physics, 1976, 65, 111-116.	1.2	718