

Simon P Webb

List of Publications by Year in descending order

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22
papers

2,169
citations

516215

16
h-index

676716

22
g-index

22
all docs

22
docs citations

22
times ranked

2117
citing authors

#	ARTICLE	IF	CITATIONS
1	An effective fragment method for modeling solvent effects in quantum mechanical calculations. <i>Journal of Chemical Physics</i> , 1996, 105, 1968-1986.	1.2	578
2	Multiconfigurational nuclear-electronic orbital approach: Incorporation of nuclear quantum effects in electronic structure calculations. <i>Journal of Chemical Physics</i> , 2002, 117, 4106-4118.	1.2	259
3	Hydride Transfer in Liver Alcohol Dehydrogenase: Quantum Dynamics, Kinetic Isotope Effects, and Role of Enzyme Motion. <i>Journal of the American Chemical Society</i> , 2001, 123, 11262-11272.	6.6	179
4	Computational Studies of the Mechanism for Proton and Hydride Transfer in Liver Alcohol Dehydrogenase. <i>Journal of the American Chemical Society</i> , 2000, 122, 4803-4812.	6.6	168
5	A derivation of the frozen-orbital unrestricted open-shell and restricted closed-shell second-order perturbation theory analytic gradient expressions. <i>Theoretical Chemistry Accounts</i> , 2003, 110, 233-253.	0.5	142
6	Determinants of the Relative Reduction Potentials of Type-1 Copper Sites in Proteins. <i>Journal of the American Chemical Society</i> , 2004, 126, 8010-8019.	6.6	134
7	Hybrid approach for including electronic and nuclear quantum effects in molecular dynamics simulations of hydrogen transfer reactions in enzymes. <i>Journal of Chemical Physics</i> , 2001, 114, 6925-6936.	1.2	121
8	Fourier grid Hamiltonian multiconfigurational self-consistent-field: A method to calculate multidimensional hydrogen vibrational wavefunctions. <i>Journal of Chemical Physics</i> , 2000, 113, 5214.	1.2	95
9	Solvation of the Menshutkin Reaction: A Rigorous Test of the Effective Fragment Method. <i>Journal of Physical Chemistry A</i> , 1999, 103, 1265-1273.	1.1	78
10	Formation of Alkali Metal/Alkaline Earth Cation Water Clusters, $M(\text{H}_2\text{O})_{1-6}$, $M = \text{Li}^+, \text{Na}^+, \text{K}^+, \text{Mg}^{2+}$, and Ca^{2+} : An Effective Fragment Potential (EFP) Case Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 386-396.	1.1	74
11	Solvent-Induced Frequency Shifts: Configuration Interaction Singles Combined with the Effective Fragment Potential Method. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6742-6750.	1.1	74
12	Modeling Protein-Ligand Binding by Mining Minima. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3540-3557.	2.3	60
13	Combining Electronic Structure Methods with the Calculation of Hydrogen Vibrational Wavefunctions: Application to Hydride Transfer in Liver Alcohol Dehydrogenase. <i>Journal of Physical Chemistry B</i> , 2000, 104, 8884-8894.	1.2	54
14	Application of the nuclear-electronic orbital method to hydrogen transfer systems: multiple centers and multiconfigurational wavefunctions. <i>Chemical Physics</i> , 2004, 304, 227-236.	0.9	40
15	Intermolecular Self-Interactions of the Titanium Tetrahalides TiX_4 ($X = \text{F}, \text{Cl}, \text{Br}$). <i>Journal of the American Chemical Society</i> , 1999, 121, 2552-2560.	6.6	28
16	Proteomic Analysis Identifies Oxidative Stress Induction by Adaphostin. <i>Clinical Cancer Research</i> , 2007, 13, 3667-3681.	3.2	22
17	The effect of spin-orbit coupling on the magnetic properties of $\text{H}_2\text{Ti}(\text{H})_2\text{TiH}_2$. <i>Journal of Chemical Physics</i> , 1998, 109, 919-927.	1.2	16
18	Molecular Electronic Structure and Energetics of the Isomers of Ti_2H_6 . <i>Journal of the American Chemical Society</i> , 1998, 120, 3846-3857.	6.6	15

#	ARTICLE	IF	CITATIONS
19	The Dimerization of TiH ₄ . Journal of the American Chemical Society, 1995, 117, 7195-7201.	6.6	9
20	Partial multidimensional grid generation method for efficient calculation of nuclear wavefunctions. Chemical Physics Letters, 2001, 338, 389-397.	1.2	9
21	Ab initio electronic structure theory as an aid to understanding excited state hydrogen transfer in moderate to large systems. Theoretical Chemistry Accounts, 2006, 116, 355-372.	0.5	8
22	Computation of host-guest binding free energies with a new quantum mechanics based mining minima algorithm. Journal of Chemical Physics, 2021, 154, 104122.	1.2	6