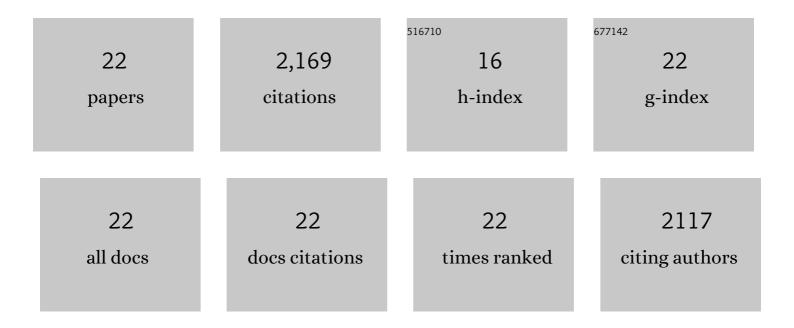
## Simon P Webb

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/9834205/publications.pdf Version: 2024-02-01



#	Article	IF	CITATIONS
1	An effective fragment method for modeling solvent effects in quantum mechanical calculations. Journal of Chemical Physics, 1996, 105, 1968-1986.	3.0	578
2	Multiconfigurational nuclear-electronic orbital approach: Incorporation of nuclear quantum effects in electronic structure calculations. Journal of Chemical Physics, 2002, 117, 4106-4118.	3.0	259
3	Hydride Transfer in Liver Alcohol Dehydrogenase:  Quantum Dynamics, Kinetic Isotope Effects, and Role of Enzyme Motion. Journal of the American Chemical Society, 2001, 123, 11262-11272.	13.7	179
4	Computational Studies of the Mechanism for Proton and Hydride Transfer in Liver Alcohol Dehydrogenase. Journal of the American Chemical Society, 2000, 122, 4803-4812.	13.7	168
5	A derivation of the frozen-orbital unrestricted open-shell and restricted closed-shell second-order perturbation theory analytic gradient expressions. Theoretical Chemistry Accounts, 2003, 110, 233-253.	1.4	142
6	Determinants of the Relative Reduction Potentials of Type-1 Copper Sites in Proteins. Journal of the American Chemical Society, 2004, 126, 8010-8019.	13.7	134
7	Hybrid approach for including electronic and nuclear quantum effects in molecular dynamics simulations of hydrogen transfer reactions in enzymes. Journal of Chemical Physics, 2001, 114, 6925-6936.	3.0	121
8	Fourier grid Hamiltonian multiconfigurational self-consistent-field: A method to calculate multidimensional hydrogen vibrational wavefunctions. Journal of Chemical Physics, 2000, 113, 5214.	3.0	95
9	Solvation of the Menshutkin Reaction:Â A Rigorous Test of the Effective Fragment Method. Journal of Physical Chemistry A, 1999, 103, 1265-1273.	2.5	78
10	Formation of Alkali Metal/Alkaline Earth Cation Water Clusters, M(H2O)1-6, M = Li+, Na+, K+, Mg2+, and Ca2+: An Effective Fragment Potential (EFP) Case Study. Journal of Physical Chemistry A, 2003, 107, 386-396.	2.5	74
11	Solvent-Induced Frequency Shifts: Configuration Interaction Singles Combined with the Effective Fragment Potential Method. Journal of Physical Chemistry A, 2010, 114, 6742-6750.	2.5	74
12	Modeling Proteinâ^'Ligand Binding by Mining Minima. Journal of Chemical Theory and Computation, 2010, 6, 3540-3557.	5.3	60
13	Combining Electronic Structure Methods with the Calculation of Hydrogen Vibrational Wavefunctions:Â Application to Hydride Transfer in Liver Alcohol Dehydrogenase. Journal of Physical Chemistry B, 2000, 104, 8884-8894.	2.6	54
14	Application of the nuclear–electronic orbital method to hydrogen transfer systems: multiple centers and multiconfigurational wavefunctions. Chemical Physics, 2004, 304, 227-236.	1.9	40
15	Intermolecular Self-Interactions of the Titanium Tetrahalides TiX4(X = F, Cl, Br). Journal of the American Chemical Society, 1999, 121, 2552-2560.	13.7	28
16	Proteomic Analysis Identifies Oxidative Stress Induction by Adaphostin. Clinical Cancer Research, 2007, 13, 3667-3681.	7.0	22
17	The effect of spin-orbit coupling on the magnetic properties of H2Ti(μ–H)2TiH2. Journal of Chemical Physics, 1998, 109, 919-927.	3.0	16
18	Molecular Electronic Structure and Energetics of the Isomers of Ti2H6. Journal of the American Chemical Society, 1998, 120, 3846-3857.	13.7	15

SIMON P WEBB

#	Article	IF	CITATIONS
19	The Dimerization of TiH4. Journal of the American Chemical Society, 1995, 117, 7195-7201.	13.7	9
20	Partial multidimensional grid generation method for efficient calculation of nuclear wavefunctions. Chemical Physics Letters, 2001, 338, 389-397.	2.6	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.	1.4	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.	3.0	6