# Simon P Webb

List of Publications by Year
in descending order



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|---|---|---|---|
| 22 papers | 2,169 citations | 516710 16 h-index | 677142 22 g-index |
| 22 all docs | 22 docs citations | 22 times ranked | 2117 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Computation of hostâ€“guest binding free energies with a new quantum mechanics based mining minima algorithm. Journal of Chemical Physics, 2021, 154, 104122. | 3.0 | 6 |
| 2 | 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 |
| 3 | Modeling Proteinâ^'Ligand Binding by Mining Minima. Journal of Chemical Theory and Computation, 2010, 6, 3540-3557. | 5.3 | 60 |
| 4 | Proteomic Analysis Identifies Oxidative Stress Induction by Adaphostin. Clinical Cancer Research, 2007, 13, 3667-3681. | 7.0 | 22 |
| 5 | 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 |
| 6 | Application of the nuclearâ€“electronic orbital method to hydrogen transfer systems: multiple centers and multiconfigurational wavefunctions. Chemical Physics, 2004, 304, 227-236. | 1.9 | 40 |
| 7 | 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 |
| 8 | 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 |
| 9 | 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 |
| 10 | 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 |
| 11 | Hydride Transfer in Liver Alcohol Dehydrogenase:â€‰ Quantum Dynamics, Kinetic Isotope Effects, and Role of Enzyme Motion. Journal of the American Chemical Society, 2001, 123, 11262-11272. | 13.7 | 179 |
| 12 | 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 |
| 13 | Partial multidimensional grid generation method for efficient calculation of nuclear wavefunctions. Chemical Physics Letters, 2001, 338, 389-397. | 2.6 | 9 |
| 14 | 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 |
| 15 | 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 |
| 16 | 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 |
| 17 | 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 |
| 18 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Molecular Electronic Structure and Energetics of the Isomers of Ti2H6. Journal of the American Chemical Society, 1998, 120, 3846-3857. | 13.7 | 15 |
| 20 | The effect of spin-orbit coupling on the magnetic properties of H2Ti(Î¼â€“H)2TiH2. Journal of Chemical Physics, 1998, 109, 919-927. | 3.0 | 16 |
| 21 | An effective fragment method for modeling solvent effects in quantum mechanical calculations. Journal of Chemical Physics, 1996, 105, 1968-1986. | 3.0 | 578 |
| 22 | The Dimerization of TiH4. Journal of the American Chemical Society, 1995, 117, 7195-7201. | 13.7 | 9 |