Michael J Frisch

List of Publications by Year in Descending Order

59 papers	28,848 citations	37 h-index	60 g-index
60 ext. papers	30,587 ext. citations	4.2 avg, IF	6.9 L-index

#	Paper	IF	Citations
59	Double hybrids and time-dependent density functional theory: An implementation and benchmark on charge transfer excited states. *Journal of Computational Chemistry*, **2020**, 41, 1242-1251	3.5	26
58	Calculation of magnetic properties with density functional approximations including rung 3.5 ingredients. *Journal of Chemical Physics*, **2020**, 153, 164101	3.9	1
57	Efficient Geometry Minimization and Transition Structure Optimization Using Interpolated Potential Energy Surfaces and Iteratively Updated Hessians. *Journal of Chemical Theory and Computation*, **2017**, 13, 6424-6432	6.4	28
56	On the Driving Force of the Excited-State Proton Shuttle in the Green Fluorescent Protein: A Time-Dependent Density Functional Theory (TD-DFT) Study of the Intrinsic Reaction Path. *Journal of Chemical Theory and Computation*, **2016**, 12, 4925-4933	6.4	25
55	Localized operator partitioning method for electronic excitation energies in the time-dependent density functional formalism. *Journal of Chemical Physics*, **2016**, 145, 244111	3.9	0
54	Density of States Guided Møller-Plesset Perturbation Theory. *Journal of Chemical Theory and Computation*, **2014**, 10, 1910-4	6.4	1
53	Quantum Calculations in Solution for Large to Very Large Molecules: A New Linear Scaling QM/Continuum Approach. *Journal of Physical Chemistry Letters*, **2014**, 5, 953-8	6.4	28
52	Quantum, classical, and hybrid QM/MM calculations in solution: general implementation of the ddCOSMO linear scaling strategy. *Journal of Chemical Physics*, **2014**, 141, 184108	3.9	37
51	Oscillator Strength: How Does TDDFT Compare to EOM-CCSD?. *Journal of Chemical Theory and Computation*, **2011**, 7, 456-66	6.4	104
50	Time-Dependent Density Functional Tight Binding: New Formulation and Benchmark of Excited States. *Journal of Chemical Theory and Computation*, **2011**, 7, 3304-13	6.4	85
49	Self-Consistent Field and Polarizable Continuum Model: A New Strategy of Solution for the Coupled Equations. *Journal of Chemical Theory and Computation*, **2011**, 7, 610-7	6.4	28
48	Basis Set Dependence of Vibrational Raman and Raman Optical Activity Intensities. *Journal of Chemical Theory and Computation*, **2011**, 7, 3323-34	6.4	104
47	Subshell fitting of relativistic atomic core electron densities for use in QTAIM analyses of ECP-based wave functions. *Journal of Physical Chemistry A*, **2011**, 115, 12879-94	2.8	39
46	Energy-Specific Linear Response TDHF/TDDFT for Calculating High-Energy Excited States. *Journal of Chemical Theory and Computation*, **2011**, 7, 3540-7	6.4	83
45	Practical computation of electronic excitation in solution: vertical excitation model. *Chemical Science*, **2011**, 2, 2143	9.4	175
44	Brueckner doubles coupled cluster method with the polarizable continuum model of solvation. *Journal of Chemical Physics*, **2011**, 134, 244113	3.9	19
43	Insights into Working Principles of Ruthenium Polypyridyl Dye-Sensitized Solar Cells from First Principles Modeling. *Journal of Physical Chemistry C*, **2011**, 115, 4297-4306	3.8	64

42	Comment on "A smooth, nonsingular, and faithful discretization scheme for polarizable continuum models: the switching/gaussian approach" [J. Chem. Phys. 133, 244111 (2010)]. *Journal of Chemical Physics*, **2011**, 134, 117101; author reply 117102	3.9	6
41	Continuous surface charge polarizable continuum models of solvation. I. General formalism. *Journal of Chemical Physics*, **2010**, 132, 114110	3.9	1701
40	A variational formulation of the polarizable continuum model. *Journal of Chemical Physics*, **2010**, 133, 014106	3.9	103
39	A Comparison of Three Variants of the Generalized Davidson Algorithm for the Partial Diagonalization of Large Non-Hermitian Matrices. *Journal of Chemical Theory and Computation*, **2010**, 6, 1966-70	6.4	14
38	Electronic Transition Energies: A Study of the Performance of a Large Range of Single Reference Density Functional and Wave Function Methods on Valence and Rydberg States Compared to Experiment. *Journal of Chemical Theory and Computation*, **2010**, 6, 370-83	6.4	181
37	Geometry Optimization with Multilayer Methods Using Least-Squares Minimization. *Journal of Chemical Theory and Computation*, **2010**, 6, 3352-7	6.4	3
36	Eigenspace Update for Molecular Geometry Optimization in Nonredundant Internal Coordinate. *Journal of Chemical Theory and Computation*, **2010**, 6, 2034-9	6.4	6
35	Coupled Cluster Calculations in Solution with the Polarizable Continuum Model of Solvation. *Journal of Physical Chemistry Letters*, **2010**, 1, 2369-2373	6.4	39
34	A theoretical study of alanine dipeptide and analogs. *International Journal of Quantum Chemistry*, **2009**, 36, 311-322	2.1	5
33	The electronic structure and electrostatics of nitrous oxide. *International Journal of Quantum Chemistry*, **2009**, 36, 363-369	2.1	0
32	An ab initio study of the structures and stabilities of the complexes of the bases N2O, CO2, and CO with the acids FH, H+, and Li+. *International Journal of Quantum Chemistry*, **2009**, 36, 371-380	2.1	2
31	Environmental effects on electronic absorption spectra using DFT: An organic and positively charged fused polycyclic chromophore as a case study. *Computational and Theoretical Chemistry*, **2009**, 914, 94-99		22
30	Relativistic interactions in the radical pair model of magnetic field sense in CRY-1 protein of Arabidopsis thaliana. *Journal of Physical Chemistry A*, **2009**, 113, 12276-84	2.8	9
29	QM:QM electronic embedding using Mulliken atomic charges: energies and analytic gradients in an ONIOM framework. *Journal of Chemical Physics*, **2008**, 128, 034107	3.9	75
28	Geometries and properties of excited states in the gas phase and in solution: theory and application of a time-dependent density functional theory polarizable continuum model. *Journal of Chemical Physics*, **2006**, 124, 94107	3.9	989
27	Energy-Represented Direct Inversion in the Iterative Subspace within a Hybrid Geometry Optimization Method. *Journal of Chemical Theory and Computation*, **2006**, 2, 835-9	6.4	324
26	Calculation of Nuclear Spin-Spin Coupling Constants of Molecules with First and Second Row Atoms in Study of Basis Set Dependence. *Journal of Chemical Theory and Computation*, **2006**, 2, 1028-37	6.4	145
25	Ab initio Ehrenfest dynamics. *Journal of Chemical Physics*, **2005**, 123, 084106	3.9	269

24	Achieving linear-scaling computational cost for the polarizable continuum model of solvation. *Theoretical Chemistry Accounts*, **2004**, 111, 90-100	1.9	112
23	Origin of the Inversion of the Acidity Order for Haloacetic Acids on Going from the Gas Phase to Solution. *Journal of Physical Chemistry A*, **2000**, 104, 7625-7628	2.8	26
22	HartreeFock and Density Functional Theory ab Initio Calculation of Optical Rotation Using GIAOs: Basis Set Dependence. *Journal of Physical Chemistry A*, **2000**, 104, 1039-1046	2.8	253
21	An efficient implementation of time-dependent density-functional theory for the calculation of excitation energies of large molecules. *Journal of Chemical Physics*, **1998**, 109, 8218-8224	3.9	4251
20	Improving harmonic vibrational frequencies calculations in density functional theory. *Journal of Chemical Physics*, **1997**, 106, 10175-10183	3.9	74
19	A comparison of models for calculating nuclear magnetic resonance shielding tensors. *Journal of Chemical Physics*, **1996**, 104, 5497-5509	3.9	1842
18	Systematic Model Chemistries Based on Density Functional Theory: Comparison with traditional Models and with Experiment. *Theoretical and Computational Chemistry*, **1996**, 4, 679-707		37
17	Using redundant internal coordinates to optimize equilibrium geometries and transition states. *Journal of Computational Chemistry*, **1996**, 17, 49-56	3.5	2353
16	A direct derivative MC-SCF procedure. *Chemical Physics Letters*, **1996**, 250, 373-378	2.5	212
15	Ab initio calculation of molar volumes: Comparison with experiment and use in solvation models. *Journal of Computational Chemistry*, **1995**, 16, 385-394	3.5	83
14	Toward a systematic molecular orbital theory for excited states. *The Journal of Physical Chemistry*, **1992**, 96, 135-149		2142
13	A fifth-order method for two-electron integral derivative transformation. *Chemical Physics Letters*, **1992**, 196, 624-629	2.5	21
12	Computational Bottlenecks in Molecular Orbital Calculations **1991**, 5-33		14
11	A direct MP2 gradient method. *Chemical Physics Letters*, **1990**, 166, 275-280	2.5	1442
10	Semi-direct algorithms for the MP2 energy and gradient. *Chemical Physics Letters*, **1990**, 166, 281-289	2.5	1131
9	MP2 energy evaluation by direct methods. *Chemical Physics Letters*, **1988**, 153, 503-506	2.5	2340
8	Analytic evaluation of infrared intensities and polarizabilities by two-configuration self-consistent field wave functions. *Theoretica Chimica Acta*, **1986**, 69, 337-352		38
7	Extensive theoretical studies of the hydrogen-bonded complexes (H2O)2, (H2O)2H+, (HF)2, (HF)2H+, F2H and (NH3)2. *Journal of Chemical Physics*, **1986**, 84, 2279-2289	3.9	621

6	Analytic Raman intensities from molecular electronic wave functions. *Journal of Chemical Physics*, **1986**, 84, 531-532	3.9	291
5	Further theoretical examination of the F + H2 entrance channel barrier. *Chemical Physics Letters*, **1985**, 114, 1-5	2.5	43
4	Self-consistent molecular orbital methods 25. Supplementary functions for Gaussian basis sets. *Journal of Chemical Physics*, **1984**, 80, 3265-3269	3.9	6545
3	Ab initio calculation of reaction energies. III. Basis set dependence of relative energies on the FH2 and H2CO potential energy surfaces. *Journal of Chemical Physics*, **1984**, 81, 1882-1893	3.9	77
2	Ab initio computation of the enthalpies of some gas-phase hydration reactions. *The Journal of Physical Chemistry*, **1983**, 87, 3279-3282		128
1	Basis set dependence of correlation corrections to protonation energies. *Chemical Physics Letters*, **1981**, 83, 240-242	2.5	31