Filippo Lipparini

List of Publications by Year in Descending Order

76 papers	2,367 citations	28 h-index	47 g-index
83 ext. papers	2,888 ext. citations	5.1 avg, IF	5.62 L-index

#	Paper	IF	Citations
76	Molecular Dynamics Simulations Enforcing Nonperiodic Boundary Conditions: New Developments and Application to the Solvent Shifts of Nitroxide Magnetic Parameters.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	2
75	The He-H complex. I. Vibration-rotation-tunneling states and transition probabilities.. *Journal of Chemical Physics*, **2022**, 156, 144307	3.9	1
74	The He-H complex. II. Infrared predissociation spectrum and energy term diagram.. *Journal of Chemical Physics*, **2022**, 156, 144308	3.9	1
73	Grassmann Extrapolation of Density Matrices for Born-Oppenheimer Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2021**, 17, 6965-6973	6.4	3
72	Second-Order CASSCF Algorithm with the Cholesky Decomposition of the Two-Electron Integrals. *Journal of Chemical Theory and Computation*, **2021**, 17, 6819-6831	6.4	1
71	Hybrid QM/classical models: Methodological advances and new applications. *Chemical Physics Reviews*, **2021**, 2, 041303	4.4	8
70	Multiscale Models for Light-Driven Processes. *Annual Review of Physical Chemistry*, **2021**, 72, 489-513	15.7	14
69	An enhanced sampling QM/AMOEBA approach: The case of the excited state intramolecular proton transfer in solvated 3-hydroxyflavone. *Journal of Chemical Physics*, **2021**, 154, 184107	3.9	8
68	How accurate are EOM-CC4 vertical excitation energies?. *Journal of Chemical Physics*, **2021**, 154, 221103	3.9	3
67	A Proline Mimetic for the Design of New Stable Secondary Structures: Solvent-Dependent Amide Bond Isomerization of ()-Indoline-2-carboxylic Acid Derivatives. *Journal of Organic Chemistry*, **2021**, 86, 7946-7954	4.2	1
66	QUESTDB: A database of highly accurate excitation energies for the electronic structure community. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1517	7.9	24
65	Is There a Quadruple Fe-C Bond in FeC(CO)3?. *Computation*, **2021**, 9, 95	2.2	
64	NMR chemical shift computations at second-order M□ller-Plesset perturbation theory using gauge-including atomic orbitals and Cholesky-decomposed two-electron integrals. *Journal of Chemical Physics*, **2021**, 155, 074105	3.9	5
63	Energy, Structures, and Response Properties with a Fully Coupled QM/AMOEBA/ddCOSMO Implementation. *Journal of Chemical Theory and Computation*, **2021**, 17, 5661-5672	6.4	3
62	Ultrafast Transient Infrared Spectroscopy of Photoreceptors with Polarizable QM/MM Dynamics. *Journal of Physical Chemistry B*, **2021**, 125, 10282-10292	3.4	3
61	From crystallographic data to the solution structure of photoreceptors: the case of the AppA BLUF domain. *Chemical Science*, **2021**, 12, 13331-13342	9.4	2
60	Fast Approximate but Accurate QM/MM Interactions for Polarizable Embedding.. *Journal of Chemical Theory and Computation*, **2021**,	6.4	1

59	Electronic Circular Dichroism Imaging (ECDi) Casts a New Light on the Origin of Solid-State Chiroptical Properties.. *Chemistry - A European Journal*, **2021**, e202103632	4.8	0
58	General formulation of polarizable embedding models and of their coupling. *Journal of Chemical Physics*, **2020**, 153, 224108	3.9	13
57	A polarisable QM/MM description of NMR chemical shifts of a photoreceptor protein. *Molecular Physics*, **2020**, 118, e1771449	1.7	5
56	Vibrational Excitation Hindering an Ion-Molecule Reaction: The c-C_{3}H_{2}^{+}-H_{2} Collision Complex. *Physical Review Letters*, **2020**, 124, 233401	7.4	12
55	Coupled-cluster techniques for computational chemistry: The CFOUR program package. *Journal of Chemical Physics*, **2020**, 152, 214108	3.9	156
54	Polarizable embedding QM/MM: the future gold standard for complex (bio)systems?. *Physical Chemistry Chemical Physics*, **2020**, 22, 14433-14448	3.6	50
53	Elucidating the role of structural fluctuations, and intermolecular and vibronic interactions in the spectroscopic response of a bacteriophytochrome. *Physical Chemistry Chemical Physics*, **2020**, 22, 8585-8594	3.6	11
52	High-resolution rovibrational spectroscopy of c-C3H2+: The ν7 CH antisymmetric stretching band. *Journal of Molecular Structure*, **2020**, 1214, 128023	3.4	4
51	An approximation strategy to compute accurate initial density matrices for repeated self-consistent field calculations at different geometries. *Molecular Physics*, **2020**, 118, e1779834	1.7	5
50	A Mountaineering Strategy to Excited States: Highly Accurate Energies and Benchmarks for Medium Sized Molecules. *Journal of Chemical Theory and Computation*, **2020**, 16, 1711-1741	6.4	63
49	The Multiple Roles of the Protein in the Photoactivation of Orange Carotenoid Protein. *CheM*, **2020**, 6, 187-203	16.2	18
48	A Many-Body, Fully Polarizable Approach to QM/MM Simulations. *Journal of Chemical Theory and Computation*, **2020**, 16, 7462-7472	6.4	7
47	Excited state Born-Oppenheimer molecular dynamics through coupling between time dependent DFT and AMOEBA. *Physical Chemistry Chemical Physics*, **2020**, 22, 19532-19541	3.6	13
46	Absorption and Circular Dichroism Spectra of Molecular Aggregates With the Full Cumulant Expansion. *Journal of Physical Chemistry B*, **2020**, 124, 8610-8617	3.4	6
45	Gas-Phase Vibrational Spectroscopy of the Hydrocarbon Cations l-CH, HCH, and c-CH: Structures, Isomers, and the Influence of Ne-Tagging. *Journal of Physical Chemistry A*, **2019**, 123, 8053-8062	2.8	20
44	Quantum Calculations in Solution of Energies, Structures, and Properties with a Domain Decomposition Polarizable Continuum Model. *Journal of Chemical Theory and Computation*, **2019**, 15, 6061-6073	6.4	8
43	Time-Dependent Complete Active Space Embedded in a Polarizable Force Field. *Journal of Chemical Theory and Computation*, **2019**, 15, 1633-1641	6.4	12
42	Accurate interaction energies by spin component scaled Møller-Plesset second order perturbation theory calculations with optimized basis sets (SCS-MP2): Development and application to aromatic heterocycles. *Journal of Chemical Physics*, **2019**, 150, 234113	3.9	6

41	Spectral Variability in Phycocyanin Cryptophyte Antenna Complexes is Controlled by Changes in the Polypeptide Chains. *ChemPhotoChem*, **2019**, 3, 945-956	3.3	8
40	Towards large scale hybrid QM/MM dynamics of complex systems with advanced point dipole polarizable embeddings. *Chemical Science*, **2019**, 10, 7200-7211	9.4	30
39	General Linear Scaling Implementation of Polarizable Embedding Schemes. *Journal of Chemical Theory and Computation*, **2019**, 15, 4312-4317	6.4	29
38	Coupled Cluster Theory with Induced Dipole Polarizable Embedding for Ground and Excited States. *Journal of Chemical Theory and Computation*, **2019**, 15, 4485-4496	6.4	8
37	Uncatalyzed conjugate addition of organozinc halides to enones in DME: a combined experimental/computational study on the role of the solvent and the reaction mechanism. *Chemical Science*, **2019**, 11, 257-263	9.4	5
36	Nonequilibrium Environment Dynamics in a Frequency-Dependent Polarizable Embedding Model. *Journal of Chemical Theory and Computation*, **2019**, 15, 43-51	6.4	15
35	Tinker-HP: a massively parallel molecular dynamics package for multiscale simulations of large complex systems with advanced point dipole polarizable force fields. *Chemical Science*, **2018**, 9, 956-972	9.4	122
34	A polarizable QM/MM description of environment effects on NMR shieldings: from solvated molecules to pigment protein complexes. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	4
33	Internally Contracted Multireference Coupled Cluster Calculations with a Spin-Free Dirac-Coulomb Hamiltonian: Application to the Monoxides of Titanium, Zirconium, and Hafnium. *Journal of Chemical Theory and Computation*, **2017**, 13, 3171-3184	6.4	7
32	Coupling Real-Time Time-Dependent Density Functional Theory with Polarizable Force Field. *Journal of Physical Chemistry Letters*, **2017**, 8, 5283-5289	6.4	18
31	Virtual Orbital Many-Body Expansions: A Possible Route towards the Full Configuration Interaction Limit. *Journal of Physical Chemistry Letters*, **2017**, 8, 4633-4639	6.4	53
30	Hybrid QM/MM Molecular Dynamics with AMOEBA Polarizable Embedding. *Journal of Chemical Theory and Computation*, **2017**, 13, 4025-4033	6.4	61
29	Computation of forces arising from the polarizable continuum model within the domain-decomposition paradigm. *Journal of Chemical Physics*, **2017**, 147, 224108	3.9	8
28	Cost-Effective Treatment of Scalar Relativistic Effects for Multireference Systems: A CASSCF Implementation Based on the Spin-free Dirac-Coulomb Hamiltonian. *Journal of Chemical Theory and Computation*, **2016**, 12, 4284-95	6.4	14
27	A new discretization for the polarizable continuum model within the domain decomposition paradigm. *Journal of Chemical Physics*, **2016**, 144, 054101	3.9	17
26	A QM/MM Approach Using the AMOEBA Polarizable Embedding: From Ground State Energies to Electronic Excitations. *Journal of Chemical Theory and Computation*, **2016**, 12, 3654-61	6.4	100
25	LICHEM: A QM/MM program for simulations with multipolar and polarizable force fields. *Journal of Computational Chemistry*, **2016**, 37, 1019-29	3.5	57
24	Perspective: Polarizable continuum models for quantum-mechanical descriptions. *Journal of Chemical Physics*, **2016**, 144, 160901	3.9	59

23	Scalable evaluation of polarization energy and associated forces in polarizable molecular dynamics: II. Toward massively parallel computations using smooth particle mesh Ewald. *Journal of Chemical Theory and Computation*, **2015**, 11, 2589-99	6.4	37
22	Achieving linear scaling in computational cost for a fully polarizable MM/continuum embedding. *Journal of Chemical Theory and Computation*, **2015**, 11, 694-704	6.4	40
21	Polarizable molecular dynamics in a polarizable continuum solvent. *Journal of Chemical Theory and Computation*, **2015**, 11, 623-34	6.4	37
20	Addressing the Issues of Non-isotropy and Non-additivity in the Development of Quantum Chemistry-Grounded Polarizable Molecular Mechanics. *Challenges and Advances in Computational Chemistry and Physics*, **2015**, 1-49	0.7	1
19	Scalable Evaluation of Polarization Energy and Associated Forces in Polarizable Molecular Dynamics: II.Towards Massively Parallel Computations using Smooth Particle Mesh Ewald. *Journal of Chemical Theory and Computation*, **2014**, 10, 1638-1651	6.4	66
18	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
17	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
16	The Optical Rotation of Methyloxirane in Aqueous Solution: A Never Ending Story?. *Journal of Chemical Theory and Computation*, **2013**, 9, 1880-4	6.4	64
15	Vertical Electronic Excitations in Solution with the EOM-CCSD Method Combined with a Polarizable Explicit/Implicit Solvent Model. *Journal of Chemical Theory and Computation*, **2013**, 9, 3035-3042	6.4	40
14	Fast Domain Decomposition Algorithm for Continuum Solvation Models: Energy and First Derivatives. *Journal of Chemical Theory and Computation*, **2013**, 9, 3637-48	6.4	64
13	A gauge invariant multiscale approach to magnetic spectroscopies in condensed phase: general three-layer model, computational implementation and pilot applications. *Journal of Chemical Physics*, **2013**, 138, 234108	3.9	42
12	Toward Ab Initio Anharmonic Vibrational Circular Dichroism Spectra in the Condensed Phase. *Journal of Physical Chemistry Letters*, **2012**, 3, 1766-73	6.4	43
11	Implementation and validation of a multi-purpose virtual spectrometer for large systems in complex environments. *Physical Chemistry Chemical Physics*, **2012**, 14, 12404-22	3.6	122
10	Linear Response Theory and Electronic Transition Energies for a Fully Polarizable QM/Classical Hamiltonian. *Journal of Chemical Theory and Computation*, **2012**, 8, 4153-65	6.4	100
9	Analytical First and Second Derivatives for a Fully Polarizable QM/Classical Hamiltonian. *Journal of Chemical Theory and Computation*, **2012**, 8, 4270-8	6.4	65
8	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
7	Polarizable Force Fields and Polarizable Continuum Model: A Fluctuating Charges/PCM Approach. 1. Theory and Implementation. *Journal of Chemical Theory and Computation*, **2011**, 7, 3711-24	6.4	126
6	Towards an accurate description of anharmonic infrared spectra in solution within the polarizable continuum model: reaction field, cavity field and nonequilibrium effects. *Journal of Chemical Physics* , **2011**, 135, 104505	3.9	45

5	A variational formulation of the polarizable continuum model. *Journal of Chemical Physics*, **2010**, 133, 014106	3.9	103
4	A fully automated implementation of VPT2 Infrared intensities. *Chemical Physics Letters*, **2010**, 496, 157-161	1.9	118
3	Non covalent interactions in RNA and DNA base pairs: a quantum-mechanical study of the coupling between solvent and electronic density. *Physical Chemistry Chemical Physics*, **2009**, 11, 11617-23	3.6	25
2	Embedding effects on charge-transport parameters in molecular organic materials. *Journal of Chemical Physics*, **2007**, 127, 144706	3.9	11
1	A black-box, general purpose quadratic self-consistent field code with and without Cholesky decomposition of the two-electron integrals. *Molecular Physics*,	1.7	1