Filippo Lipparini

List of Publications by Year
in descending order

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80 papers	3,406 citations	147786 31 h-index	149686 56 g-index
83 all docs	83 docs citations	83 times ranked	2535 citing authors

#	Article	IF	Citations
1	Coupled-cluster techniques for computational chemistry: The <scp>CFOUR</scp> program package. Journal of Chemical Physics, 2020, 152, 214108.	3.0	375
2	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.	7.4	190
3	A fully automated implementation of VPT2 Infrared intensities. Chemical Physics Letters, 2010, 496, 157-161.	2.6	140
4	A QM/MM Approach Using the AMOEBA Polarizable Embedding: From Ground State Energies to Electronic Excitations. Journal of Chemical Theory and Computation, 2016, 12, 3654-3661.	5.3	136
5	Polarizable Force Fields and Polarizable Continuum Model: A Fluctuating Charges/PCM Approach. 1. Theory and Implementation. Journal of Chemical Theory and Computation, 2011, 7, 3711-3724.	5.3	135
6	Implementation and validation of a multi-purpose virtual spectrometer for large systems in complex environments. Physical Chemistry Chemical Physics, 2012, 14, 12404.	2.8	128
7	A variational formulation of the polarizable continuum model. Journal of Chemical Physics, 2010, 133, 014106.	3.0	125
8	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.	5.3	119
9	Linear Response Theory and Electronic Transition Energies for a Fully Polarizable QM/Classical Hamiltonian. Journal of Chemical Theory and Computation, 2012, 8, 4153-4165.	5.3	111
10	Polarizable embedding QM/MM: the future gold standard for complex (bio)systems?. Physical Chemistry Chemical Physics, 2020, 22, 14433-14448.	2.8	109
11	<scp>QUESTDB</scp>: A database of highly accurate excitation energies for the electronic structure community. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1517.	14.6	84
12	Fast Domain Decomposition Algorithm for Continuum Solvation Models: Energy and First Derivatives. Journal of Chemical Theory and Computation, 2013, 9, 3637-3648.	5.3	81
13	Perspective: Polarizable continuum models for quantum-mechanical descriptions. Journal of Chemical Physics, 2016, 144, 160901.	3.0	81
14	Hybrid QM/MM Molecular Dynamics with AMOEBA Polarizable Embedding. Journal of Chemical Theory and Computation, 2017, 13, 4025-4033.	5.3	81
15	The Optical Rotation of Methyloxirane in Aqueous Solution: A Never Ending Story?. Journal of Chemical Theory and Computation, 2013, 9, 1880-1884.	5.3	76
16	Scalable Evaluation of Polarization Energy and Associated Forces in Polarizable Molecular Dynamics: I. Toward Massively Parallel Direct Space Computations. Journal of Chemical Theory and Computation, 2014, 10, 1638-1651.	5.3	76
17	Analytical First and Second Derivatives for a Fully Polarizable QM/Classical Hamiltonian. Journal of Chemical Theory and Computation, 2012, 8, 4270-4278.	5.3	68
18	<scp>LICHEM</scp>: A <scp>QM</scp>/<scp>MM</scp> program for simulations with multipolar and polarizable force fields. Journal of Computational Chemistry, 2016, 37, 1019-1029.	3.3	68

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19	Virtual Orbital Many-Body Expansions: A Possible Route towards the Full Configuration Interaction Limit. Journal of Physical Chemistry Letters, 2017, 8, 4633-4639.	4.6	60
20	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, 2589-2599.	5.3	53
21	Toward Ab Initio Anharmonic Vibrational Circular Dichroism Spectra in the Condensed Phase. Journal of Physical Chemistry Letters, 2012, 3, 1766-1773.	4.6	50
22	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.	3.0	48
23	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.	5.3	48
24	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.	3.0	47
25	Quantum, classical, and hybrid QM/MM calculations in solution: General implementation of the ddCOSMO linear scaling strategy. Journal of Chemical Physics, 2014, 141, 184108.	3.0	47
26	Achieving Linear Scaling in Computational Cost for a Fully Polarizable MM/Continuum Embedding. Journal of Chemical Theory and Computation, 2015, 11, 694-704.	5.3	45
27	Polarizable Molecular Dynamics in a Polarizable Continuum Solvent. Journal of Chemical Theory and Computation, 2015, 11, 623-634.	5.3	45
28	Towards large scale hybrid QM/MM dynamics of complex systems with advanced point dipole polarizable embeddings. Chemical Science, 2019, 10, 7200-7211.	7.4	45
29	General Linear Scaling Implementation of Polarizable Embedding Schemes. Journal of Chemical Theory and Computation, 2019, 15, 4312-4317.	5.3	39
30	The Multiple Roles of the Protein in the Photoactivation of Orange Carotenoid Protein. CheM, 2020, 6, 187-203.	11.7	39
31	Gas-Phase Vibrational Spectroscopy of the Hydrocarbon Cations l-C₃H⁺, HC₃H⁺, and c-C₃H₂⁺: Structures, Isomers, and the Influence of Ne-Tagging. Journal of Physical Chemistry A, 2019, 123, 8053-8062.	2.5	33
32	Quantum Calculations in Solution for Large to Very Large Molecules: A New Linear Scaling QM/Continuum Approach. Journal of Physical Chemistry Letters, 2014, 5, 953-958.	4.6	32
33	Self-Consistent Field and Polarizable Continuum Model: A New Strategy of Solution for the Coupled Equations. Journal of Chemical Theory and Computation, 2011, 7, 610-617.	5.3	31
34	Multiscale Models for Light-Driven Processes. Annual Review of Physical Chemistry, 2021, 72, 489-513.	10.8	29
35	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.	2.8	27
36	Hybrid QM/classical models: Methodological advances and new applications. Chemical Physics Reviews, 2021, 2, .	5.7	26

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37	Coupling Real-Time Time-Dependent Density Functional Theory with Polarizable Force Field. Journal of Physical Chemistry Letters, 2017, 8, 5283-5289.	4.6	25
38	Nonequilibrium Environment Dynamics in a Frequency-Dependent Polarizable Embedding Model. Journal of Chemical Theory and Computation, 2019, 15, 43-51.	5.3	24
39	Cost-Effective Treatment of Scalar Relativistic Effects for Multireference Systems: A CASSCF Implementation Based on the Spin-free Diracâ€“Coulomb Hamiltonian. Journal of Chemical Theory and Computation, 2016, 12, 4284-4295.	5.3	19
40	A new discretization for the polarizable continuum model within the domain decomposition paradigm. Journal of Chemical Physics, 2016, 144, 054101.	3.0	19
41	Excited state Bornâ€“Oppenheimer molecular dynamics through coupling between time dependent DFT and AMOEBA. Physical Chemistry Chemical Physics, 2020, 22, 19532-19541.	2.8	19
42	Vibrational Excitation Hindering an Ion-Molecule Reaction: The <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">c</mml:mi><mml:mtext>â^'</mml:mtext><mml:msub><mml:mrow><mml:mi mathvariant="normal">C</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub><mml:msup><mml:m mathvariant="normal">H</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow><mml:n Physical Review Letters, 2020, 124, 233401.	7.8	19
43	How to make continuum solvation incredibly fast in a few simple steps: A practical guide to the domain decomposition paradigm for the conductorâ€like screening model. International Journal of Quantum Chemistry, 2019, 119, e25669.	2.0	17
44	Absorption and Circular Dichroism Spectra of Molecular Aggregates With the Full Cumulant Expansion. Journal of Physical Chemistry B, 2020, 124, 8610-8617.	2.6	17
45	General formulation of polarizable embedding models and of their coupling. Journal of Chemical Physics, 2020, 153, 224108.	3.0	17
46	Time-Dependent Complete Active Space Embedded in a Polarizable Force Field. Journal of Chemical Theory and Computation, 2019, 15, 1633-1641.	5.3	16
47	Spectral Variability in Phycocyanin Cryptophyte Antenna Complexes is Controlled by Changes in the Î±â€Polypeptide Chains. ChemPhotoChem, 2019, 3, 945-956.	3.0	15
48	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.	2.8	15
49	How accurate are EOM-CC4 vertical excitation energies?. Journal of Chemical Physics, 2021, 154, 221103.	3.0	14
50	Coupled Cluster Theory with Induced Dipole Polarizable Embedding for Ground and Excited States. Journal of Chemical Theory and Computation, 2019, 15, 4485-4496.	5.3	13
51	NMR chemical shift computations at second-order MÃ¸llerâ€“Plesset perturbation theory using gauge-including atomic orbitals and Cholesky-decomposed two-electron integrals. Journal of Chemical Physics, 2021, 155, 074105.	3.0	12
52	Second-Order CASSCF Algorithm with the Cholesky Decomposition of the Two-Electron Integrals. Journal of Chemical Theory and Computation, 2021, 17, 6819-6831.	5.3	12
53	A Mountaineering Strategy to Excited States: Revising Reference Values with EOM-CC4. Journal of Chemical Theory and Computation, 2022, 18, 4418-4427.	5.3	12
54	Embedding effects on charge-transport parameters in molecular organic materials. Journal of Chemical Physics, 2007, 127, 144706.	3.0	11

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55	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.	5.3	11
56	A Many-Body, Fully Polarizable Approach to QM/MM Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7462-7472.	5.3	11
57	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	11
58	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.	3.0	11
59	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, 2020, 11, 257-263.	7.4	10
60	Grassmann Extrapolation of Density Matrices for Bornâ€“Oppenheimer Molecular Dynamics. Journal of Chemical Theory and Computation, 2021, 17, 6965-6973.	5.3	10
61	Computation of forces arising from the polarizable continuum model within the domain-decomposition paradigm. Journal of Chemical Physics, 2017, 147, 224108.	3.0	9
62	A polarisable QM/MM description of NMR chemical shifts of a photoreceptor protein. Molecular Physics, 2020, 118, e1771449.	1.7	9
63	Ultrafast Transient Infrared Spectroscopy of Photoreceptors with Polarizable QM/MM Dynamics. Journal of Physical Chemistry B, 2021, 125, 10282-10292.	2.6	9
64	From crystallographic data to the solution structure of photoreceptors: the case of the AppA BLUF domain. Chemical Science, 2021, 12, 13331-13342.	7.4	9
65	A polarizable QM/MM description of environment effects on NMR shieldings: from solvated molecules to pigmentâ€“protein complexes. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	8
66	Accurate interaction energies by spin component scaled MÃ¶ller-Plesset second order perturbation theory calculations with optimized basis sets (SCS-MP2 mod): Development and application to aromatic heterocycles. Journal of Chemical Physics, 2019, 150, 234113.	3.0	8
67	Energy, Structures, and Response Properties with a Fully Coupled QM/AMOEBA/ddCOSMO Implementation. Journal of Chemical Theory and Computation, 2021, 17, 5661-5672.	5.3	8
68	A black-box, general purpose quadratic self-consistent field code with and without Cholesky decomposition of the two-electron integrals. Molecular Physics, 2021, 119, .	1.7	8
69	Internally Contracted Multireference Coupled Cluster Calculations with a Spin-Free Diracâ€“Coulomb Hamiltonian: Application to the Monoxides of Titanium, Zirconium, and Hafnium. Journal of Chemical Theory and Computation, 2017, 13, 3171-3184.	5.3	7
70	Fast Approximate but Accurate QM/MM Interactions for Polarizable Embedding. Journal of Chemical Theory and Computation, 2022, 18, 344-356.	5.3	6
71	Electronic Circular Dichroism Imaging (ECDi) Casts a New Light on the Origin of Solidâ€State Chiroptical Properties. Chemistry - A European Journal, 2022, 28, e202103632.	3.3	6
72	High-resolution rovibrational spectroscopy of c-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:mrow><mml:msub><mml:mtext>C</mml:mtext><mml:mn>3</mml:mn></mml:msub><mml:msubsup><mml:m The <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.svg"><mml:mrow><mml:msub><mml:mi>Î½</mml:mi><mml:mn>7</mml:mn></mml:msub></mml:mrow></mml:math> Câ€“H antisymmetric stretching band. Journal of Molecular Structure, 2020, 1214, 128023.	3.6	5

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73	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, , .	5.3	5
74	Probing aqueous ions with non-local Auger relaxation. Physical Chemistry Chemical Physics, 2022, 24, 8661-8671.	2.8	4
75	A Î”SCF model for excited states within a polarisable embedding. Molecular Physics, 0, , .	1.7	4
76	A Proline Mimetic for the Design of New Stable Secondary Structures: Solvent-Dependent Amide Bond Isomerization of (S)-Indoline-2-carboxylic Acid Derivatives. Journal of Organic Chemistry, 2021, 86, 7946-7954.	3.2	3
77	The Heâ€“H3+ complex. II. Infrared predissociation spectrum and energy term diagram. Journal of Chemical Physics, 2022, 156, 144308.	3.0	3
78	The Heâ€“H3+ complex. I. Vibration-rotation-tunneling states and transition probabilities. Journal of Chemical Physics, 2022, 156, 144307.	3.0	2
79	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.	0.6	1
80	Is There a Quadruple Fe-C Bond in FeC(CO)3?. Computation, 2021, 9, 95.	2.0	0