

# Srinivasan S Iyengar

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

71  
papers

2,989  
citations

25  
h-index

54  
g-index

72  
ext. papers

3,232  
ext. citations

4  
avg, IF

5.1  
L-index

#	Paper	IF	Citations
71	Graph-Theory-Based Molecular Fragmentation for Efficient and Accurate Potential Surface Calculations in Multiple Dimensions. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 6671-6690	6.4	1
70	Mapping Quantum Chemical Dynamics Problems to Spin-Lattice Simulators. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 6713-6732	6.4	1
69	Weighted-Graph-Theoretic Methods for Many-Body Corrections within ONIOM: Smooth AIMD and the Role of High-Order Many-Body Terms. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 2672-2690	6.4	2
68	Embedded, graph-theoretically defined many-body approximations for wavefunction-in-DFT and DFT-in-DFT: Applications to gas- and condensed-phase ab initio molecular dynamics, and potential surfaces for quantum nuclear effects. <i>International Journal of Quantum Chemistry</i> , <b>2020</b> , 120, e26244	2.1	4
67	Efficient and Accurate Approach To Estimate Hybrid Functional and Large Basis-Set Contributions to Condensed-Phase Systems and Molecule-Surface Interactions. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 4790-4812	6.4	2
66	Adaptive Dimensional Decoupling for Compression of Quantum Nuclear Wave Functions and Efficient Potential Energy Surface Representations through Tensor Network Decomposition. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 2780-2796	6.4	5
65	Fragment-Based Electronic Structure for Potential Energy Surfaces Using a Superposition of Fragmentation Topologies. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 5769-5786	6.4	6
64	Emerging opportunities and future directions: general discussion. <i>Faraday Discussions</i> , <b>2019</b> , 221, 564-581	3.6	5
63	Zero-point energy and tunnelling: general discussion. <i>Faraday Discussions</i> , <b>2019</b> , 221, 478-500	3.6	4
62	Photoelectrons Are Not Always Quite Free. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 144-149	6.4	7
61	Challenges in constructing accurate methods for hydrogen transfer reactions in large biological assemblies: rare events sampling for mechanistic discovery and tensor networks for quantum nuclear effects. <i>Faraday Discussions</i> , <b>2019</b> , 221, 379-405	3.6	2
60	Exotic electronic structures of SmCeO ( $x = 0-3$ ; $y = 2-4$ ) clusters and the effect of high neutral density of low-lying states on photodetachment transition intensities. <i>Journal of Chemical Physics</i> , <b>2018</b> , 149, 054305	3.9	12
59	Efficient and Adaptive Methods for Computing Accurate Potential Surfaces for Quantum Nuclear Effects: Applications to Hydrogen-Transfer Reactions. <i>Journal of Chemical Theory and Computation</i> , <b>2018</b> , 14, 30-47	6.4	10
58	Efficiently Capturing Weak Interactions in ab Initio Molecular Dynamics with on-the-Fly Basis Set Extrapolation. <i>Journal of Chemical Theory and Computation</i> , <b>2018</b> , 14, 5535-5552	6.4	8
57	Adaptive, Geometric Networks for Efficient Coarse-Grained Ab Initio Molecular Dynamics with Post-Hartree-Fock Accuracy. <i>Journal of Chemical Theory and Computation</i> , <b>2018</b> , 14, 2852-2866	6.4	11
56	Efficient, "On-the-Fly", Born-Oppenheimer and Car-Parrinello-type Dynamics with Coupled Cluster Accuracy through Fragment Based Electronic Structure. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 1887-1901	6.4	16
55	Proton relays in anomalous carbocations dictate spectroscopy, stability, and mechanisms: case studies on CH and CH. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 27801-27816	3.6	5

54	The electron shuffle: Cerium influences samarium 4f orbital occupancy in heteronuclear Ce-Sm oxide clusters. <i>Journal of Chemical Physics</i> , <b>2017</b> , 146, 194310	3.9	14
53	A Grotthuss-like proton shuttle in the anomalous CH carbocation: energetic and vibrational properties for isotopologues. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 29395-29411	3.6	10
52	Hybrid Extended Lagrangian, Post-Hartree-Fock Born-Oppenheimer ab Initio Molecular Dynamics Using Fragment-Based Electronic Structure. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 2493-508	6.4	25
51	Active Site Dynamical Effects in the Hydrogen Transfer Rate-limiting Step in the Catalysis of Linoleic Acid by Soybean Lipoxygenase-1 (SLO-1): Primary and Secondary Isotope Contributions. <i>Journal of Physical Chemistry B</i> , <b>2015</b> , 119, 9532-46	3.4	15
50	Ab Initio Molecular Dynamics Using Recursive, Spatially Separated, Overlapping Model Subsystems Mixed within an ONIOM-Based Fragmentation Energy Extrapolation Technique. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 3978-91	6.4	20
49	Teaching Thermodynamics and Kinetics to Advanced General Chemistry Students and to Upper-Level Undergraduate Students Using PV Diagrams. <i>Journal of Chemical Education</i> , <b>2014</b> , 91, 74-83 <sup>2,4</sup>		3
48	Vibrational Properties of Hydrogen-Bonded Systems Using the Multireference Generalization to the "On-the-Fly" Electronic Structure within Quantum Wavepacket ab Initio Molecular Dynamics (QWAIMD). <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 2265-80	6.4	11
47	A Multiwavelet Treatment of the Quantum Subsystem in Quantum Wavepacket Ab Initio Molecular Dynamics through an Hierarchical Partitioning of Momentum Space. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 2950-63	6.4	7
46	Using Quantum Mechanics To Facilitate the Introduction of a Broad Range of Chemical Concepts to First-Year Undergraduate Students. <i>Journal of Chemical Education</i> , <b>2013</b> , 90, 717-725	2.4	11
45	Constructing Periodic Phase Space Orbits from ab Initio Molecular Dynamics Trajectories to Analyze Vibrational Spectra: Case Study of the Zundel (H <sub>5</sub> O <sub>2</sub> <sup>+</sup> ) Cation. <i>Journal of Chemical Theory and Computation</i> , <b>2012</b> , 8, 4876-90	6.4	17
44	Influence of water on anharmonicity, stability, and vibrational energy distribution of hydrogen-bonded adducts in atmospheric reactions: case study of the OH + isoprene reaction intermediate using ab initio molecular dynamics. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 399-414	2.8	23
43	"Pump-probe" atom-centered density matrix propagation studies to gauge anharmonicity and energy repartitioning in atmospheric reactive adducts: case study of the OH + isoprene and OH + butadiene reaction intermediates. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 4108-28	2.8	9
42	Gauging the flexibility of the active site in soybean lipoxygenase-1 (SLO-1) through an atom-centered density matrix propagation (ADMP) treatment that facilitates the sampling of rare events. <i>Journal of Physical Chemistry B</i> , <b>2012</b> , 116, 10145-64	3.4	21
41	Quantum wavepacket ab initio molecular dynamics for extended systems. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 6269-84	2.8	15
40	Shannon Entropy Based Time-Dependent Deterministic Sampling for Efficient "On-the-Fly" Quantum Dynamics and Electronic Structure. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 256-68	6.4	13
39	Multistage ab initio quantum wavepacket dynamics for electronic structure and dynamics in open systems: momentum representation, coupled electron-nuclear dynamics, and external fields. <i>Journal of Chemical Physics</i> , <b>2011</b> , 134, 074107	3.9	8
38	Isotope dependent, temperature regulated, energy repartitioning in a low-barrier, short-strong hydrogen bonded cluster. <i>Journal of Chemical Physics</i> , <b>2010</b> , 132, 244301	3.9	43
37	Quantum wavepacket ab initio molecular dynamics: generalizations using an extended Lagrangian treatment of diabatic states coupled through multireference electronic structure. <i>Journal of Chemical Physics</i> , <b>2010</b> , 133, 184105	3.9	14

36	Analysis of Hydrogen Tunneling in an Enzyme Active Site using von Neumann Measurements. <i>Journal of Chemical Theory and Computation</i> , <b>2010</b> , 6, 6-10	6.4	17
35	A multistage ab initio quantum wavepacket dynamics formalism for electronic structure and dynamics in open systems. <i>Journal of Chemical Physics</i> , <b>2010</b> , 133, 044105	3.9	13
34	Computing vibrational properties in hydrogen-bonded systems using quantum wavepacket ab initio molecular dynamics. <i>International Journal of Quantum Chemistry</i> , <b>2009</b> , 109, 3798-3810	2.1	11
33	Hydrogen tunneling in an enzyme active site: a quantum wavepacket dynamical perspective. <i>Journal of Physical Chemistry B</i> , <b>2008</b> , 112, 7601-13	3.4	58
32	The Study of Dynamically Averaged Vibrational Spectroscopy of Atmospherically Relevant Clusters Using Ab Initio Molecular Dynamics in Conjunction with Quantum Wavepackets. <i>Advances in Quantum Chemistry</i> , <b>2008</b> , 55, 333-353	1.4	7
31	Experimental and ab initio dynamical investigations of the kinetics and intramolecular energy transfer mechanisms for the OH + 1,3-butadiene reaction between 263 and 423 K at low pressure. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 7227-37	2.8	28
30	Multiscale theory of collective and quasiparticle modes in quantum nanosystems. <i>Journal of Chemical Physics</i> , <b>2008</b> , 128, 164716	3.9	7
29	Insights from first principles molecular dynamics studies toward infrared multiple-photon and single-photon action spectroscopy: case study of the proton-bound dimethyl ether dimer. <i>Journal of Chemical Physics</i> , <b>2008</b> , 128, 184308	3.9	54
28	Combining quantum wavepacket ab initio molecular dynamics with QM/MM and QM/QM techniques: Implementation blending ONIOM and empirical valence bond theory. <i>Journal of Chemical Physics</i> , <b>2008</b> , 129, 054109	3.9	25
27	Can the four-coordinated, penta-valent oxygen in hydroxide water clusters be detected through experimental vibrational spectroscopy?. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 4815-20	2.8	41
26	Quantum wavepacket ab initio molecular dynamics: an approach for computing dynamically averaged vibrational spectra including critical nuclear quantum effects. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 10313-24	2.8	52
25	Further analysis of the dynamically averaged vibrational spectrum for the "magic" protonated 21-water cluster. <i>Journal of Chemical Physics</i> , <b>2007</b> , 126, 216101	3.9	48
24	Ab initio dynamics with wave-packets and density matrices. <i>Theoretical Chemistry Accounts</i> , <b>2006</b> , 116, 326-337	1.9	26
23	The properties of ion-water clusters. II. Solvation structures of Na <sup>+</sup> , Cl <sup>-</sup> , and H <sup>+</sup> clusters as a function of temperature. <i>Journal of Chemical Physics</i> , <b>2006</b> , 124, 024327	3.9	64
22	Computational Improvements to Quantum Wave Packet ab Initio Molecular Dynamics Using a Potential-Adapted, Time-Dependent Deterministic Sampling Technique. <i>Journal of Chemical Theory and Computation</i> , <b>2006</b> , 2, 1203-19	6.4	30
21	Dynamical effects on vibrational and electronic spectra of hydroperoxyl radical water clusters. <i>Journal of Chemical Physics</i> , <b>2005</b> , 123, 084310	3.9	45
20	The properties of ion-water clusters. I. The protonated 21-water cluster. <i>Journal of Chemical Physics</i> , <b>2005</b> , 123, 084309	3.9	149
19	On the amphiphilic behavior of the hydrated proton: an ab initio molecular dynamics study. <i>International Journal of Mass Spectrometry</i> , <b>2005</b> , 241, 197-204	1.9	93

18	Comment on "Curvy-steps approach to constraint-free extended-Lagrangian ab initio molecular dynamics, using atom-centered basis functions: convergence toward Born-Oppenheimer trajectories" [J. Chem. Phys. 121, 11542 (2004)]. <i>Journal of Chemical Physics</i> , <b>2005</b> , 123, 27101; author reply 027102	3.9	5
17	Quantum wave packet ab initio molecular dynamics: an approach to study quantum dynamics in large systems. <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 114105	3.9	49
16	Effect of time-dependent basis functions and their superposition error on atom-centered density matrix propagation (ADMP): connections to wavelet theory of multiresolution analysis. <i>Journal of Chemical Physics</i> , <b>2004</b> , 121, 5061-70	3.9	56
15	The Hydrated Proton at the Water Liquid/Vapor Interface. <i>Journal of Physical Chemistry B</i> , <b>2004</b> , 108, 14804-14806	3.4	237
14	Hybrid Ab-Initio/Empirical Molecular Dynamics: Combining the ONIOM Scheme with the Atom-Centered Density Matrix Propagation (ADMP) Approach. <i>Journal of Physical Chemistry B</i> , <b>2004</b> , 108, 4210-4220	3.4	115
13	Atom-Centered Density Matrix Propagation (ADMP): Generalizations Using Bohmian Mechanics□	2.8	49
12	Modeling condensed-phase chemistry through molecular dynamics simulation. <i>Computing in Science and Engineering</i> , <b>2003</b> , 5, 31-35	1.5	4
11	Quantum reactive scattering in three dimensions using adiabatically adjusting principal axis hyperspherical coordinates: Periodic distributed approximating functional method for surface functions. <i>Journal of Chemical Physics</i> , <b>2003</b> , 118, 569-581	3.9	2
10	Ab initio molecular dynamics: Propagating the density matrix with gaussian orbitals. IV. Formal analysis of the deviations from born-oppenheimer dynamics. <i>Israel Journal of Chemistry</i> , <b>2002</b> , 42, 191-202	3.4	63
9	Ab initio molecular dynamics: Propagating the density matrix with Gaussian orbitals. III. Comparison with BornOppenheimer dynamics. <i>Journal of Chemical Physics</i> , <b>2002</b> , 117, 8694-8704	3.9	361
8	Challenge of creating accurate and effective kinetic-energy functionals. <i>Physical Review A</i> , <b>2001</b> , 63,	2.6	34
7	Ab initio molecular dynamics: Propagating the density matrix with Gaussian orbitals. <i>Journal of Chemical Physics</i> , <b>2001</b> , 114, 9758-9763	3.9	436
6	Ab initio molecular dynamics: Propagating the density matrix with Gaussian orbitals. II. Generalizations based on mass-weighting, idempotency, energy conservation and choice of initial conditions. <i>Journal of Chemical Physics</i> , <b>2001</b> , 115, 10291	3.9	320
5	Bounding the extrapolated correlation energy using Padéapproximants. <i>International Journal of Quantum Chemistry</i> , <b>2000</b> , 79, 222-234	2.1	12
4	Particular and homogeneous solutions of time-independent wavepacket Schrödinger equations: calculations using a subset of eigenstates of undamped or damped Hamiltonians. <i>Theoretical Chemistry Accounts</i> , <b>2000</b> , 104, 471-483	1.9	15
3	Estimating bounds on the highest and lowest eigenvalues of any matrix. <i>Theoretical Chemistry Accounts</i> , <b>2000</b> , 103, 507-517	1.9	4
2	Symmetry-adapted distributed approximating functionals: Theory and application to the ro-vibrational states of H3+. <i>Journal of Chemical Physics</i> , <b>1999</b> , 110, 10283-10298	3.9	17
1	Further analysis of solutions to the time-independent wave packet equations of quantum dynamics. II. Scattering as a continuous function of energy using finite, discrete approximate Hamiltonians. <i>Journal of Chemical Physics</i> , <b>1996</b> , 105, 927-939	3.9	62

