Srinivasan S Iyengar

List of Publications by Citations

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	Ab initio molecular dynamics: Propagating the density matrix with Gaussian orbitals. *Journal of Chemical Physics*, **2001**, 114, 9758-9763	3.9	436
70	Ab initio molecular dynamics: Propagating the density matrix with Gaussian orbitals. III. Comparison with Born□Oppenheimer dynamics. *Journal of Chemical Physics*, **2002**, 117, 8694-8704	3.9	361
69	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. *Journal of Chemical Physics*, **2001**, 115, 10291	3.9	320
68	The Hydrated Proton at the Water Liquid/Vapor Interface. *Journal of Physical Chemistry B*, **2004**, 108, 14804-14806	3.4	237
67	The properties of ion-water clusters. I. The protonated 21-water cluster. *Journal of Chemical Physics* , **2005**, 123, 084309	3.9	149
66	Hybrid Ab-Initio/Empirical Molecular Dynamics: Combining the ONIOM Scheme with the Atom-Centered Density Matrix Propagation (ADMP) Approach. *Journal of Physical Chemistry B*, **2004**, 108, 4210-4220	3.4	115
65	On the amphiphilic behavior of the hydrated proton: an ab initio molecular dynamics study. *International Journal of Mass Spectrometry*, **2005**, 241, 197-204	1.9	93
64	The properties of ion-water clusters. II. Solvation structures of Na+, Cl-, and H+ clusters as a function of temperature. *Journal of Chemical Physics*, **2006**, 124, 024327	3.9	64
63	Ab initio molecular dynamics: Propagating the density matrix with gaussian orbitals. IV. Formal analysis of the deviations from born-oppenheimer dynamics. *Israel Journal of Chemistry*, **2002**, 42, 191-202	3.4	63
62	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. *Journal of Chemical Physics*, **1996**, 105, 927-939	3.9	62
61	Hydrogen tunneling in an enzyme active site: a quantum wavepacket dynamical perspective. *Journal of Physical Chemistry B*, **2008**, 112, 7601-13	3.4	58
60	Effect of time-dependent basis functions and their superposition error on atom-centered density matrix propagation (ADMP): connections to wavelet theory of multiresolution analysis. *Journal of Chemical Physics*, **2004**, 121, 5061-70	3.9	56
59	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. *Journal of Chemical Physics*, **2008**, 128, 184308	3.9	54
58	Quantum wavepacket ab initio molecular dynamics: an approach for computing dynamically averaged vibrational spectra including critical nuclear quantum effects. *Journal of Physical Chemistry A*, **2007**, 111, 10313-24	2.8	52
57	Atom-Centered Density Matrix Propagation (ADMP): Generalizations Using Bohmian Mechanics□ *Journal of Physical Chemistry A*, **2003**, 107, 7269-7277	2.8	49
56	Quantum wave packet ab initio molecular dynamics: an approach to study quantum dynamics in large systems. *Journal of Chemical Physics*, **2005**, 122, 114105	3.9	49
55	Further analysis of the dynamically averaged vibrational spectrum for the "magic" protonated 21-water cluster. *Journal of Chemical Physics*, **2007**, 126, 216101	3.9	48

54	Dynamical effects on vibrational and electronic spectra of hydroperoxyl radical water clusters. *Journal of Chemical Physics*, **2005**, 123, 084310	3.9	45
53	Isotope dependent, temperature regulated, energy repartitioning in a low-barrier, short-strong hydrogen bonded cluster. *Journal of Chemical Physics*, **2010**, 132, 244301	3.9	43
52	Can the four-coordinated, penta-valent oxygen in hydroxide water clusters be detected through experimental vibrational spectroscopy?. *Journal of Physical Chemistry A*, **2007**, 111, 4815-20	2.8	41
51	Challenge of creating accurate and effective kinetic-energy functionals. *Physical Review A*, **2001**, 63,	2.6	34
50	Computational Improvements to Quantum Wave Packet ab Initio Molecular Dynamics Using a Potential-Adapted, Time-Dependent Deterministic Sampling Technique. *Journal of Chemical Theory and Computation*, **2006**, 2, 1203-19	6.4	30
49	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. *Journal of Physical Chemistry A*, **2008**, 112, 7227-37	2.8	28
48	Ab initio dynamics with wave-packets and density matrices. *Theoretical Chemistry Accounts*, **2006**, 116, 326-337	1.9	26
47	Combining quantum wavepacket ab initio molecular dynamics with QM/MM and QM/QM techniques: Implementation blending ONIOM and empirical valence bond theory. *Journal of Chemical Physics*, **2008**, 129, 054109	3.9	25
46	Hybrid Extended Lagrangian, Post-Hartree-Fock Born-Oppenheimer ab Initio Molecular Dynamics Using Fragment-Based Electronic Structure. *Journal of Chemical Theory and Computation*, **2016**, 12, 2493-508	6.4	25
45	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. *Journal of Physical Chemistry A*, **2012**, 116, 399-414	2.8	23
44	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. *Journal of Physical Chemistry B*, **2012**, 116, 10145-64	3.4	21
43	Ab Initio Molecular Dynamics Using Recursive, Spatially Separated, Overlapping Model Subsystems Mixed within an ONIOM-Based Fragmentation Energy Extrapolation Technique. *Journal of Chemical Theory and Computation*, **2015**, 11, 3978-91	6.4	20
42	Constructing Periodic Phase Space Orbits from ab Initio Molecular Dynamics Trajectories to Analyze Vibrational Spectra: Case Study of the Zundel (H5O2(+)) Cation. *Journal of Chemical Theory and Computation*, **2012**, 8, 4876-90	6.4	17
41	Analysis of Hydrogen Tunneling in an Enzyme Active Site using von Neumann Measurements. *Journal of Chemical Theory and Computation*, **2010**, 6, 6-10	6.4	17
40	Symmetry-adapted distributed approximating functionals: Theory and application to the ro-vibrational states of H3+. *Journal of Chemical Physics*, **1999**, 110, 10283-10298	3.9	17
39	Efficient, "On-the-Fly", Born-Oppenheimer and Car-Parrinello-type Dynamics with Coupled Cluster Accuracy through Fragment Based Electronic Structure. *Journal of Chemical Theory and Computation*, **2017**, 13, 1887-1901	6.4	16
38	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. *Journal of Physical Chemistry B*, **2015**, 119, 9532-46	3.4	15
37	Quantum wavepacket ab initio molecular dynamics for extended systems. *Journal of Physical Chemistry A*, **2011**, 115, 6269-84	2.8	15

36	Particular and homogeneous solutions of time-independent wavepacket Schr□dinger equations: calculations using a subset of eigenstates of undamped or damped Hamiltonians. *Theoretical Chemistry Accounts*, **2000**, 104, 471-483	1.9	15
35	The electron shuffle: Cerium influences samarium 4f orbital occupancy in heteronuclear Ce-Sm oxide clusters. *Journal of Chemical Physics*, **2017**, 146, 194310	3.9	14
34	Quantum wavepacket ab initio molecular dynamics: generalizations using an extended Lagrangian treatment of diabatic states coupled through multireference electronic structure. *Journal of Chemical Physics*, **2010**, 133, 184105	3.9	14
33	A multistage ab initio quantum wavepacket dynamics formalism for electronic structure and dynamics in open systems. *Journal of Chemical Physics*, **2010**, 133, 044105	3.9	13
32	Shannon Entropy Based Time-Dependent Deterministic Sampling for Efficient "On-the-Fly" Quantum Dynamics and Electronic Structure. *Journal of Chemical Theory and Computation*, **2011**, 7, 256-68	6.4	13
31	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. *Journal of Chemical Physics*, **2018**, 149, 054305	3.9	12
30	Bounding the extrapolated correlation energy using Pad□approximants. *International Journal of Quantum Chemistry*, **2000**, 79, 222-234	2.1	12
29	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). *Journal of Chemical Theory and Computation*, **2014**, 10, 2265-80	6.4	11
28	Using Quantum Mechanics To Facilitate the Introduction of a Broad Range of Chemical Concepts to First-Year Undergraduate Students. *Journal of Chemical Education*, **2013**, 90, 717-725	2.4	11
27	Computing vibrational properties in hydrogen-bonded systems using quantum wavepacket ab initio molecular dynamics. *International Journal of Quantum Chemistry*, **2009**, 109, 3798-3810	2.1	11
26	Adaptive, Geometric Networks for Efficient Coarse-Grained Ab Initio Molecular Dynamics with Post-Hartree-Fock Accuracy. *Journal of Chemical Theory and Computation*, **2018**, 14, 2852-2866	6.4	11
25	A Grotthuss-like proton shuttle in the anomalous CH carbocation: energetic and vibrational properties for isotopologues. *Physical Chemistry Chemical Physics*, **2016**, 18, 29395-29411	3.6	10
24	Efficient and Adaptive Methods for Computing Accurate Potential Surfaces for Quantum Nuclear Effects: Applications to Hydrogen-Transfer Reactions. *Journal of Chemical Theory and Computation*, **2018**, 14, 30-47	6.4	10
23	"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. *Journal of Physical Chemistry A*, **2012**, 116, 4108-28	2.8	9
22	Multistage ab initio quantum wavepacket dynamics for electronic structure and dynamics in open systems: momentum representation, coupled electron-nuclear dynamics, and external fields. *Journal of Chemical Physics*, **2011**, 134, 074107	3.9	8
21	Efficiently Capturing Weak Interactions in ab Initio Molecular Dynamics with on-the-Fly Basis Set Extrapolation. *Journal of Chemical Theory and Computation*, **2018**, 14, 5535-5552	6.4	8
20	A Multiwavelet Treatment of the Quantum Subsystem in Quantum Wavepacket Ab Initio Molecular Dynamics through an Hierarchical Partitioning of Momentum Space. *Journal of Chemical Theory and Computation*, **2014**, 10, 2950-63	6.4	7
19	The Study of Dynamically Averaged Vibrational Spectroscopy of Atmospherically Relevant Clusters Using Ab Initio Molecular Dynamics in Conjunction with Quantum Wavepackets. *Advances in Quantum Chemistry*, **2008**, 55, 333-353	1.4	7

18	Multiscale theory of collective and quasiparticle modes in quantum nanosystems. *Journal of Chemical Physics*, **2008**, 128, 164716	3.9	7
17	Photoelectrons Are Not Always Quite Free. *Journal of Physical Chemistry Letters*, **2019**, 10, 144-149	6.4	7
16	Fragment-Based Electronic Structure for Potential Energy Surfaces Using a Superposition of Fragmentation Topologies. *Journal of Chemical Theory and Computation*, **2019**, 15, 5769-5786	6.4	6
15	Adaptive Dimensional Decoupling for Compression of Quantum Nuclear Wave Functions and Efficient Potential Energy Surface Representations through Tensor Network Decomposition. *Journal of Chemical Theory and Computation*, **2019**, 15, 2780-2796	6.4	5
14	Proton relays in anomalous carbocations dictate spectroscopy, stability, and mechanisms: case studies on CH and CH. *Physical Chemistry Chemical Physics*, **2017**, 19, 27801-27816	3.6	5
13	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)]. *Journal of Chemical Physics*, **2005**, 123, 27101; author reply 027102	3.9	5
12	Emerging opportunities and future directions: general discussion. *Faraday Discussions*, **2019**, 221, 564-581	3.6	5
11	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. *International Journal of Quantum Chemistry*, **2020**, 120, e26244	2.1	4
10	Modeling condensed-phase chemistry through molecular dynamics simulation. *Computing in Science and Engineering*, **2003**, 5, 31-35	1.5	4
9	Estimating bounds on the highest and lowest eigenvalues of any matrix. *Theoretical Chemistry Accounts*, **2000**, 103, 507-517	1.9	4
8	Zero-point energy and tunnelling: general discussion. *Faraday Discussions*, **2019**, 221, 478-500	3.6	4
7	Teaching Thermodynamics and Kinetics to Advanced General Chemistry Students and to Upper-Level Undergraduate Students Using PV Diagrams. *Journal of Chemical Education*, **2014**, 91, 74-83	2.4	3
6	Efficient and Accurate Approach To Estimate Hybrid Functional and Large Basis-Set Contributions to Condensed-Phase Systems and Molecule-Surface Interactions. *Journal of Chemical Theory and Computation*, **2020**, 16, 4790-4812	6.4	2
5	Quantum reactive scattering in three dimensions using adiabatically adjusting principal axis hyperspherical coordinates: Periodic distributed approximating functional method for surface functions. *Journal of Chemical Physics*, **2003**, 118, 569-581	3.9	2
4	Weighted-Graph-Theoretic Methods for Many-Body Corrections within ONIOM: Smooth AIMD and the Role of High-Order Many-Body Terms. *Journal of Chemical Theory and Computation*, **2021**, 17, 2672-2690	6.4	2
3	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. *Faraday Discussions*, **2019**, 221, 379-405	3.6	2
2	Graph-Theory-Based Molecular Fragmentation for Efficient and Accurate Potential Surface Calculations in Multiple Dimensions. *Journal of Chemical Theory and Computation*, **2021**, 17, 6671-6690	6.4	1
1	Mapping Quantum Chemical Dynamics Problems to Spin-Lattice Simulators. *Journal of Chemical Theory and Computation*, **2021**, 17, 6713-6732	6.4	1