Sara Bonella

List of Publications by Year
in descending order

55 papers	1,183 citations	586496 16 h-index	445137 33 g-index
56 all docs	56 docs citations	56 times ranked	926 citing authors

#	Article	IF	Citations
1	Simulation of Nuclear Quantum Effects in Condensed Matter Systems via Quantum Baths. Applied Sciences (Switzerland), 2022, 12, 4756.	1.3	6
2	Fluctuation Relations for Dissipative Systems in Constant External Magnetic Field: Theory and Molecular Dynamics Simulations. Entropy, 2021, 23, 146.	1.1	6
3	Mass-Zero constrained dynamics and statistics for the shell model in magnetic field. European Physical Journal B, 2021, 94, 1.	0.6	3
4	Nuclear Quantum Effects in Liquid Water at Near Classical Computational Cost Using the Adaptive Quantum Thermal Bath. Journal of Physical Chemistry Letters, 2021, 12, 8285-8291.	2.1	17
5	Anharmonic spectral features via trajectory-based quantum dynamics: A perturbative analysis of the interplay between dynamics and sampling. Journal of Chemical Physics, 2021, 155, 104108.	1.2	18
6	Charge fluctuations from molecular simulations in the constant-potential ensemble. Physical Chemistry Chemical Physics, 2020, 22, 10480-10489.	1.3	53
7	Fluctuation relations for systems in a constant magnetic field. Physical Review E, 2020, 102, 030101.	0.8	8
8	Mass-zero constrained molecular dynamics for electrode charges in simulations of electrochemical systems. Journal of Chemical Physics, 2020, 152, 194701.	1.2	16
9	Adiabatic motion and statistical mechanics via mass-zero constrained dynamics. Physical Chemistry Chemical Physics, 2020, 22, 10775-10785.	1.3	15
10	MetalWalls: A classical molecular dynamics software dedicated to the simulation of electrochemical systems. Journal of Open Source Software, 2020, 5, 2373.	2.0	56
11	The Fluctuationâ€“Dissipation Theorem as a Diagnosis and Cure for Zero-Point Energy Leakage in Quantum Thermal Bath Simulations. Journal of Chemical Theory and Computation, 2019, 15, 2863-2880.	2.3	19
12	Sampling the thermal Wigner density via a generalized Langevin dynamics. Journal of Chemical Physics, 2019, 151, 114114.	1.2	9
13	Communication: Constrained molecular dynamics for polarizable models. Journal of Chemical Physics, 2018, 149, 191102.	1.2	16
14	Time reversal and symmetries of time correlation functions. Molecular Physics, 2018, 116, 3097-3103.	0.8	13
15	Fermi resonance in CO2: Mode assignment and quantum nuclear effects from first principles molecular dynamics. Journal of Chemical Physics, 2017, 146, 134102.	1.2	19
16	Thermal Diffusion in Binary Mixtures: Transient Behavior and Transport Coefficients from Equilibrium and Nonequilibrium Molecular Dynamics. Langmuir, 2017, 33, 11281-11290.	1.6	15
17	Time-reversal symmetry for systems in a constant external magnetic field. Physical Review E, 2017, 96, 012160.	0.8	14
18	Quantum Correlations under Time Reversal and Incomplete Parity Transformations in the Presence of a Constant Magnetic Field. Symmetry, 2017, 9, 120.	1.1	4

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19	Characterization of the Photochemical Properties of 5-Benzyluracil via Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2017, 121, 3909-3917.	1.1	15
20	Charge transport in superionic and melted AgI under a magnetic field studied via molecular dynamics. Physical Review B, 2016, 94, .	1.1	11
21	On the establishment of thermal diffusion in binary Lennard-Jones liquids. European Physical Journal: Special Topics, 2016, 225, 1629-1642.	1.2	9
22	Probabilistic Derivation of Spatiotemporal Correlation Functions in the Hydrodynamic Limit. Journal of Physical Chemistry B, 2016, 120, 1996-2000.	1.2	2
23	Gas phase infrared spectra from quasi-classical Kubo time correlation functions. Molecular Physics, 2015, 113, 2894-2904.	0.8	4
24	An introduction to the problem of bridging quantum and classical dynamics. European Physical Journal: Special Topics, 2015, 224, 2305-2320.	1.2	3
25	Time reversal symmetry in time-dependent correlation functions for systems in a constant magnetic field. Europhysics Letters, 2014, 108, 60004.	0.7	19
26	Computing thermal Wigner densities with the phase integration method. Journal of Chemical Physics, 2014, 141, 084102.	1.2	15
27	Mapping the Hydropathy of Amino Acids Based on Their Local Solvation Structure. Journal of Physical Chemistry B, 2014, 118, 6604-6613.	1.2	13
28	Photophysics and Photochemistry of a DNAâ€“Protein Cross-Linking Model: A Synergistic Approach Combining Experiments and Theory. Journal of Physical Chemistry B, 2014, 118, 4983-4992.	1.2	15
29	Gas phase infrared spectra via the phase integration quasi-classical method. Molecular Simulation, 2014, 40, 196-207.	0.9	3
30	Charge transport simulations of NaCl in an external magnetic field: the quest for the Hall effect. Molecular Physics, 2013, 111, 3651-3661.	0.8	7
31	Quantum dynamical structure factor of liquid neon via a quasiclassical symmetrized method. Journal of Chemical Physics, 2013, 138, 054118.	1.2	11
32	Early Stage of the Dehydrogenation of NaAlH₄ by Ab Initio Rare Event Simulations. Journal of Physical Chemistry C, 2012, 116, 19636-19643.	1.5	14
33	Silver self aggregation in a nanodevice for enhanced Raman spectroscopy: experiments vs. simplified modeling via molecular dynamics. Nanoscale, 2012, 4, 2362.	2.8	7
34	The quantum free energy barrier for hydrogen vacancy diffusion in Na3AlH6. Physical Chemistry Chemical Physics, 2012, 14, 15458.	1.3	3
35	Short range hydrogen diffusion in Na3AlH6. Physical Chemistry Chemical Physics, 2011, 13, 10546.	1.3	6
36	Linearized symmetrized quantum time correlation functions calculation via phase pre-averaging. Molecular Physics, 2011, 109, 3015-3027.	0.8	13

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37	Linearized approximations for condensed phase non-adiabatic dynamics: Multi-layered baths and Brownian dynamics implementation. Chemical Physics, 2010, 370, 87-97.	0.9	17
38	Linearization approximations and Liouville quantumâ€“classical dynamics. Chemical Physics Letters, 2010, 484, 399-404.	1.2	38
39	Analysis of the quantum-classical Liouville equation in the mapping basis. Journal of Chemical Physics, 2010, 133, 134115.	1.2	60
40	Path integral based calculations of symmetrized time correlation functions. II. Journal of Chemical Physics, 2010, 133, 164105.	1.2	15
41	Hydration Structure of the Quaternary Ammonium Cations. Journal of Physical Chemistry B, 2010, 114, 15018-15028.	1.2	31
42	SDPhound, a Mutual Information-Based Method to Investigate Specificity-Determining Positions. Algorithms, 2009, 2, 764-789.	1.2	2
43	Modified single sweep method for reconstructing free-energy landscapes. Molecular Simulation, 2009, 35, 1116-1129.	0.9	13
44	Iterative linearized approach to nonadiabatic dynamics. Journal of Chemical Physics, 2008, 129, 114106.	1.2	67
45	An Adiabatic Linearized Path Integral Approach for Quantum Time-Correlation Functions II:Â A Cumulant Expansion Method for Improving Convergence. Journal of Physical Chemistry B, 2006, 110, 16026-16034.	1.2	6
46	Linearized, time-dependent, non-adiabatic quantum correlation functions. Computer Physics Communications, 2005, 169, 267-273.	3.0	4
47	LAND-map, a linearized approach to nonadiabatic dynamics using the mapping formalism. Journal of Chemical Physics, 2005, 122, 194102.	1.2	134
48	Linearized path integral approach for calculating nonadiabatic time correlation functions. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6715-6719.	3.3	68
49	Trajectory Study of Supercollision Relaxation in Highly Vibrationally Excited Pyrazine and CO2. Journal of Physical Chemistry A, 2005, 109, 7657-7666.	1.1	34
50	An Adiabatic Linearized Path Integral Approach for Quantum Time Correlation Functions:Â Electronic Transport in Metalâ^'Molten Salt Solutionsâ€. Journal of Physical Chemistry B, 2005, 109, 6855-6865.	1.2	25
51	Semiclassical implementation of the mapping Hamiltonian approach for nonadiabatic dynamics using focused initial distribution sampling. Journal of Chemical Physics, 2003, 118, 4370-4385.	1.2	75
52	Semi-classical implementation of mapping Hamiltonian methods for general non-adiabatic problems. Chemical Physics, 2001, 268, 189-200.	0.9	32
53	A semiclassical limit for the mapping Hamiltonian approach to electronically nonadiabatic dynamics. Journal of Chemical Physics, 2001, 114, 7778-7789.	1.2	72
54	Vibrational Dynamics of the I3Radical:Â A Semiempirical Potential Surface, and Semiclassical Calculation of the Anion Photoelectron Spectrum. Journal of Physical Chemistry A, 1999, 103, 9552-9563.	1.1	12

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55	The semiclassical limit of the intermediate scattering function. Molecular Physics, 1996, 89, 1203-1207.	0.8	1