Mariana Rossi

List of Publications by Year
in descending order

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52 papers	2,315 citations	186209 28 h-index	206029 48 g-index
52 all docs	52 docs citations	52 times ranked	3047 citing authors

#	Article	IF	Citations
1	Dispersion Interactions with Density-Functional Theory: Benchmarking Semiempirical and Interatomic Pairwise Corrected Density Functionals. Journal of Chemical Theory and Computation, 2011, 7, 3944-3951.	2.3	265
2	i-PI 2.0: A universal force engine for advanced molecular simulations. Computer Physics Communications, 2019, 236, 214-223.	3.0	220
3	How to remove the spurious resonances from ring polymer molecular dynamics. Journal of Chemical Physics, 2014, 140, 234116.	1.2	174
4	Semiconducting Nanowireâ€Based Optoelectronic Fibers. Advanced Materials, 2017, 29, 1700681.	11.1	116
5	Isomer-Selective Detection of Hydrogen-Bond Vibrations in the Protonated Water Hexamer. Journal of the American Chemical Society, 2013, 135, 8266-8273.	6.6	107
6	Designing Real Nanotube-Based Gas Sensors. Physical Review Letters, 2008, 100, 176803.	2.9	102
7	Unraveling the Stability of Polypeptide Helices: Critical Role of van der Waals Interactions. Physical Review Letters, 2011, 106, 118102.	2.9	97
8	Secondary Structure of Ac-Ala_n-LysH⁺ Polyalanine Peptides (n =) Tj ETQq0 0 0 rgBT /Overlock 1	2.1	76
9	Communication: On the consistency of approximate quantum dynamics simulation methods for vibrational spectra in the condensed phase. Journal of Chemical Physics, 2014, 141, 181101.	1.2	74
10	Elucidating the Nuclear Quantum Dynamics of Intramolecular Double Hydrogen Transfer in Porphycene. Journal of the American Chemical Society, 2019, 141, 2526-2534.	6.6	68
11	Anharmonic and Quantum Fluctuations in Molecular Crystals: A First-Principles Study of the Stability of Paracetamol. Physical Review Letters, 2016, 117, 115702.	2.9	59
12	Fine tuning classical and quantum molecular dynamics using a generalized Langevin equation. Journal of Chemical Physics, 2018, 148, 102301.	1.2	52
13	Nuclear Quantum Effects in H⁺ and OH^{â€“} Diffusion along Confined Water Wires. Journal of Physical Chemistry Letters, 2016, 7, 3001-3007.	2.1	50
14	Exploring the conformational preferences of 20-residue peptides in isolation: Ac-Ala₁₉-Lys + H⁺vs. Ac-Lys-Ala₁₉ + H⁺ and the current reach of DFT. Physical Chemistry Chemical Physics, 2015, 17, 7373-7385.	1.3	48
15	Inverse Temperature Dependence of Nuclear Quantum Effects in DNA Base Pairs. Journal of Physical Chemistry Letters, 2016, 7, 2125-2131.	2.1	46
16	Using Gaussian process regression to simulate the vibrational Raman spectra of molecular crystals. New Journal of Physics, 2019, 21, 105001.	1.2	44
17	Validation Challenge of Density-Functional Theory for Peptidesâ€”Example of Ac-Phe-Ala₅-LysH⁺. Journal of Physical Chemistry A, 2014, 118, 7349-7359.	1.1	43
18	Stability of Complex Biomolecular Structures: van der Waals, Hydrogen Bond Cooperativity, and Nuclear Quantum Effects. Journal of Physical Chemistry Letters, 2015, 6, 4233-4238.	2.1	43

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19	Properties of the water to boron nitride interaction: From zero to two dimensions with benchmark accuracy. Journal of Chemical Physics, 2017, 147, 044710.	1.2	43
20	Role of methyl-induced polarization in ion binding. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 12978-12983.	3.3	42
21	All-electron, real-space perturbation theory for homogeneous electric fields: theory, implementation, and application within DFT. New Journal of Physics, 2018, 20, 073040.	1.2	36
22	Impact of Vibrational Entropy on the Stability of Unsolvated Peptide Helices with Increasing Length. Journal of Physical Chemistry B, 2013, 117, 5574-5584.	1.2	35
23	Activation Energy of Organic Cation Rotation in CH₃NH₃PbI₃ and CD₃NH₃PbI₃: Quasi-Elastic Neutron Scattering Measurements and First-Principles Analysis Including Nuclear Quantum Effects. Journal of Physical Chemistry Letters, 2018, 9, 3969-3977.	2.1	34
24	Decisive role of nuclear quantum effects on surface mediated water dissociation at finite temperature. Journal of Chemical Physics, 2018, 148, 102320.	1.2	32
25	Assessment of Approximate Methods for Anharmonic Free Energies. Journal of Chemical Theory and Computation, 2019, 15, 5845-5857.	2.3	31
26	Nuclear dynamics of singlet exciton fission in pentacene single crystals. Science Advances, 2021, 7, .	4.7	31
27	Modulation of the Work Function by the Atomic Structure of Strong Organic Electron Acceptors on Hâ€Si(111). Advanced Electronic Materials, 2019, 5, 1800891.	2.6	30
28	Going clean: structure and dynamics of peptides in the gas phase and paths to solvation. Journal of Physics Condensed Matter, 2015, 27, 493002.	0.7	29
29	Quantum tunneling in real space: Tautomerization of single porphycene molecules on the (111) surface of Cu, Ag, and Au. Journal of Chemical Physics, 2018, 148, 102330.	1.2	29
30	Learning Electron Densities in the Condensed Phase. Journal of Chemical Theory and Computation, 2021, 17, 7203-7214.	2.3	24
31	Temperature dependence of the vibrational spectrum of porphycene: a qualitative failure of classical-nuclei molecular dynamics. Faraday Discussions, 2020, 221, 526-546.	1.6	22
32	Water Adsorption at Two Unsolvated Peptides with a Protonated Lysine Residue: From Self-Solvation to Solvation. Journal of Physical Chemistry B, 2012, 116, 14788-14804.	1.2	20
33	Anharmonic effects in the low-frequency vibrational modes of aspirin and paracetamol crystals. Physical Review Materials, 2019, 3, .	0.9	20
34	Realistic calculations of carbon-based disordered systems. Journal Physics D: Applied Physics, 2010, 43, 374002.	1.3	19
35	Characterization of a transâ€“trans Carbonic Acidâ€“Fluoride Complex by Infrared Action Spectroscopy in Helium Nanodroplets. Journal of the American Chemical Society, 2019, 141, 5815-5823.	6.6	18
36	Progress and challenges in ab initio simulations of quantum nuclei in weakly bonded systems. Journal of Chemical Physics, 2021, 154, 170902.	1.2	15

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37	Pentacene and tetracene molecules and films on H/Si(111): level alignment from hybrid density functional theory. Electronic Structure, 2020, 2, 035002.	1.0	15
38	Native like helices in a specially designed Î² peptide in the gas phase. Physical Chemistry Chemical Physics, 2015, 17, 5376-5385.	1.3	14
39	Charge Transfer-Mediated Dramatic Enhancement of Raman Scattering upon Molecular Point Contact Formation. Nano Letters, 2022, 22, 2170-2176.	4.5	14
40	Ultrafast charge transfer and vibronic coupling in a laser-excited hybrid inorganic/organic interface. Advances in Physics: X, 2020, 5, 1749883.	1.5	12
41	Temperatureâ€Dependent Electronic Groundâ€State Charge Transfer in van der Waals Heterostructures. Advanced Materials, 2021, 33, e2008677.	11.1	12
42	Real-Space Observation of Quantum Tunneling by a Carbon Atom: Flipping Reaction of Formaldehyde on Cu(110). Journal of Physical Chemistry Letters, 2019, 10, 645-649.	2.1	9
43	The conformational space of a flexible amino acid at metallic surfaces. International Journal of Quantum Chemistry, 2021, 121, e26369.	1.0	9
44	Multidimensional Hydrogen Tunneling in Supported Molecular Switches: The Role of Surface Interactions. Physical Review Letters, 2020, 125, 216001.	2.9	6
45	Quantum Nuclei at Weakly Bonded Interfaces: The Case of Cyclohexane on Rh(111). Advanced Theory and Simulations, 2021, 4, 2000241.	1.3	6
46	Dissipative tunneling rates through the incorporation of first-principles electronic friction in instanton rate theory. I. Theory. Journal of Chemical Physics, 2022, 156, .	1.2	6
47	Emerging opportunities and future directions: general discussion. Faraday Discussions, 2019, 221, 564-581.	1.6	5
48	Efficient Gaussian process regression for prediction of molecular crystals harmonic free energies. Npj Computational Materials, 2021, 7, .	3.5	5
49	Zero-point energy and tunnelling: general discussion. Faraday Discussions, 2019, 221, 478-500.	1.6	4
50	Dissipative tunneling rates through the incorporation of first-principles electronic friction in instanton rate theory. II. Benchmarks and applications. Journal of Chemical Physics, 2022, 156, .	1.2	4
51	Van der Waals Heterostructures: Temperatureâ€Dependent Electronic Groundâ€State Charge Transfer in van der Waals Heterostructures (Adv. Mater. 29/2021). Advanced Materials, 2021, 33, 2170229.	11.1	0
52	Cover Image, Volume 121, Issue 3. International Journal of Quantum Chemistry, 2021, 121, e26284.	1.0	0