Simone Meloni

List of Publications by Year
in descending order

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84 papers	4,342 citations	172457 29 h-index	110387 64 g-index
91 all docs	91 docs citations	91 times ranked	6919 citing authors

#	Article	IF	Citations
1	Double Life of Methanol: Experimental Studies and Nonequilibrium Molecular-Dynamics Simulation of Methanol Effects on Methane-Hydrate Nucleation. Journal of Physical Chemistry C, 2022, 126, 6075-6081.	3.1	9
2	Subnanometer Topological Tuning of the Liquid Intrusion/Extrusion Characteristics of Hydrophobic Micropores. Nano Letters, 2022, 22, 2164-2169.	9.1	11
3	Wavefunction-Based Electrostatic-Embedding QM/MM Using CFOUR through MiMiC. Journal of Chemical Theory and Computation, 2022, 18, 13-24.	5.3	2
4	Kinetics and energeticsÂof metal halide perovskite conversion reactions at the nanoscale. Communications Materials, 2022, 3, .	6.9	12
5	Intrusion and extrusion of liquids in highly confining media: bridging fundamental research to applications. Advances in Physics: X, 2022, 7, .	4.1	9
6	Turning Molecular Springs into Nano-Shock Absorbers: The Effect of Macroscopic Morphology and Crystal Size on the Dynamic Hysteresis of Water Intrusionâ€“Extrusion into-from Hydrophobic Nanopores. ACS Applied Materials & Interfaces, 2022, 14, 26699-26713.	8.0	10
7	Effect of the Topology on Wetting and Drying of Hydrophobic Porous Materials. ACS Applied Materials & Interfaces, 2022, 14, 30067-30079.	8.0	6
8	Giant Negative Compressibility by Liquid Intrusion into Superhydrophobic Flexible Nanoporous Frameworks. Nano Letters, 2021, 21, 2848-2853.	9.1	24
9	Crystalâ€Sizeâ€Induced Band Gap Tuning in Perovskite Films. Angewandte Chemie - International Edition, 2021, 60, 21368-21376.	13.8	28
10	Crystalâ€Sizeâ€Induced Band Gap Tuning in Perovskite Films. Angewandte Chemie, 2021, 133, 21538-21546.	2.0	10
11	Liquid intrusion in and extrusion from non-wettable nanopores for technological applications. European Physical Journal B, 2021, 94, 1.	1.5	18
12	Halide Versus Nonhalide Salts: The Effects of Guanidinium Salts on the Structural, Morphological, and Photovoltaic Performances of Perovskite Solar Cells. Solar Rrl, 2020, 4, 1900234.	5.8	19
13	Accuracy of Molecular Simulation-Based Predictions of k_{off} Values: A Metadynamics Study. Journal of Physical Chemistry Letters, 2020, 11, 6373-6381.	4.6	41
14	The interplay among gas, liquid and solid interactions determines the stability of surface nanobubbles. Nanoscale, 2020, 12, 22698-22709.	5.6	27
15	Defect Dynamics in MAPbI₃ Polycrystalline Films: The Trapping Effect of Grain Boundaries. Helvetica Chimica Acta, 2020, 103, e2000110.	1.6	10
16	Atomistic Origins of the Limited Phase Stability of Cs⁺-Rich FA_xCs_(1â€“x)PbI₃ Mixtures. Chemistry of Materials, 2020, 32, 2605-2614.	6.7	24
17	MiMiC: Multiscale Modeling in Computational Chemistry. Frontiers in Molecular Biosciences, 2020, 7, 45.	3.5	5
18	Molecular Basis of CLC Antiporter Inhibition by Fluoride. Journal of the American Chemical Society, 2020, 142, 7254-7258.	13.7	20

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19	The Role of Grain Boundaries on Ionic Defect Migration in Metal Halide Perovskites. Advanced Energy Materials, 2020, 10, 1903735.	19.5	117
20	Hydrophilicity and Water Contact Angle on Methylammonium Lead Iodide. Advanced Materials Interfaces, 2019, 6, 1801173.	3.7	43
21	Extreme Scalability of DFT-Based QM/MM MD Simulations Using MiMiC. Journal of Chemical Theory and Computation, 2019, 15, 5601-5613.	5.3	32
22	MiMiC: A Novel Framework for Multiscale Modeling in Computational Chemistry. Journal of Chemical Theory and Computation, 2019, 15, 3810-3823.	5.3	31
23	How far does the defect tolerance of lead-halide perovskites range? The example of Bi impurities introducing efficient recombination centers. Journal of Materials Chemistry A, 2019, 7, 23838-23853.	10.3	57
24	Dual effect of humidity on cesium lead bromide: enhancement and degradation of perovskite films. Journal of Materials Chemistry A, 2019, 7, 12292-12302.	10.3	74
25	Wetting and recovery of nano-patterned surfaces beyond the classical picture. Nanoscale, 2019, 11, 21458-21470.	5.6	14
26	Pore Morphology Determines Spontaneous Liquid Extrusion from Nanopores. ACS Nano, 2019, 13, 1728-1738.	14.6	25
27	Pressure control in interfacial systems: Atomistic simulations of vapor nucleation. Journal of Chemical Physics, 2018, 148, 064706.	3.0	19
28	Self-Recovery Superhydrophobic Surfaces: Modular Design. ACS Nano, 2018, 12, 359-367.	14.6	29
29	Activated Wetting of Nanostructured Surfaces: Reaction Coordinates, Finite Size Effects, and Simulation Pitfalls. Journal of Physical Chemistry B, 2018, 122, 200-212.	2.6	11
30	Viscosity at the Nanoscale: Confined Liquid Dynamics and Thermal Effects in Self-Recovering Nanobumpers. Journal of Physical Chemistry C, 2018, 122, 14248-14256.	3.1	15
31	Intrusion and extrusion of a liquid on nanostructured surfaces. Journal of Physics Condensed Matter, 2017, 29, 014003.	1.8	18
32	Mechanisms and Nucleation Rate of Methane Hydrate by Dynamical Nonequilibrium Molecular Dynamics. Journal of Physical Chemistry C, 2017, 121, 24223-24234.	3.1	30
33	Computational Characterization of the Dependence of Halide Perovskite Effective Masses on Chemical Composition and Structure. Journal of Physical Chemistry C, 2017, 121, 23886-23895.	3.1	38
34	Collective Molecular Mechanisms in the CH₃NH₃PbI₃ Dissolution by Liquid Water. ACS Nano, 2017, 11, 9183-9190.	14.6	73
35	Collapse of superhydrophobicity on nanopillared surfaces. Physical Review Fluids, 2017, 2, .	2.5	19
36	Focus Article: Theoretical aspects of vapor/gas nucleation at structured surfaces. Journal of Chemical Physics, 2016, 145, 211802.	3.0	37

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37	Extended Intermolecular Interactions Governing Photocurrentâ€“Voltage Relations in Ternary Organic Solar Cells. Journal of Physical Chemistry Letters, 2016, 7, 3936-3944.	4.6	11
38	Valence and conduction band tuning in halide perovskites for solar cell applications. Journal of Materials Chemistry A, 2016, 4, 15997-16002.	10.3	132
39	Origin of unusual bandgap shift and dual emission in organic-inorganic lead halide perovskites. Science Advances, 2016, 2, e1601156.	10.3	307
40	Ionic polarization-induced currentâ€“voltage hysteresis in CH3NH3PbX3 perovskite solar cells. Nature Communications, 2016, 7, 10334.	12.8	602
41	Entropic stabilization of mixed A-cation ABX₃ metal halide perovskites for high performance perovskite solar cells. Energy and Environmental Science, 2016, 9, 656-662.	30.8	1,077
42	Mechanism of the Cassie-Wenzel transition via the atomistic and continuum string methods. Journal of Chemical Physics, 2015, 142, 104701.	3.0	35
43	Unraveling the Salvinia Paradox: Design Principles for Submerged Superhydrophobicity. Advanced Materials Interfaces, 2015, 2, 1500248.	3.7	39
44	Free energies for rare events: Temperature accelerated MD and MC. European Physical Journal: Special Topics, 2015, 224, 2389-2407.	2.6	10
45	Clathrate structure-type recognition: Application to hydrate nucleation and crystallisation. Journal of Chemical Physics, 2015, 142, 244503.	3.0	33
46	10.1063/1.4913839.5. , 2015, , .		0
47	Nucleation of silicon nanoparticles in amorphous silicon dioxide matrices. , 2014, , .		2
48	Massively parallel molecular dynamics simulation of formation of clathrate-hydrate precursors at planar water-methane interfaces: Insights into heterogeneous nucleation. Journal of Chemical Physics, 2014, 140, 204714.	3.0	56
49	Relaxation of a steep density gradient in a simple fluid: Comparison between atomistic and continuum modeling. Journal of Chemical Physics, 2014, 141, 154107.	3.0	10
50	Methane Clathrate Hydrate Nucleation Mechanism by Advanced Molecular Simulations. Journal of Physical Chemistry C, 2014, 118, 22847-22857.	3.1	87
51	An observable for vacancy characterization and diffusion in crystals. Journal of Chemical Physics, 2013, 138, 144103.	3.0	5
52	Probing the Structures of Hydrated Nafion in Different Morphologies Using Temperature-Accelerated Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2013, 117, 774-782.	3.1	17
53	Equilibrium and Rate Constants, and Reaction Mechanism of the HF Dissociation in the HF(H₂O)₇ Cluster by ab Initio Rare Event Simulations. Journal of Physical Chemistry A, 2013, 117, 13039-13050.	2.5	13
54	Geometry as a Catalyst: How Vapor Cavities Nucleate from Defects. Langmuir, 2013, 29, 14873-14884.	3.5	49

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55	Early Stage of the Dehydrogenation of NaAlH₄ by Ab Initio Rare Event Simulations. Journal of Physical Chemistry C, 2012, 116, 19636-19643.	3.1	14
56	Theory and methods for rare events. European Physical Journal B, 2012, 85, 1.	1.5	43
57	The influence of silicon nanoclusters on the optical properties of a-SiNx samples: A theoretical study. Applied Physics Letters, 2012, 100, 181905.	3.3	11
58	Metastable Wetting on Superhydrophobic Surfaces: Continuum and Atomistic Views of the Cassie-Baxterâ€“Wenzel Transition. Physical Review Letters, 2012, 109, 226102.	7.8	131
59	Cassieâ€“Baxter and Wenzel States on a Nanostructured Surface: Phase Diagram, Metastabilities, and Transition Mechanism by Atomistic Free Energy Calculations. Langmuir, 2012, 28, 10764-10772.	3.5	179
60	Hydrodynamics from statistical mechanics: combined dynamical-NEMD and conditional sampling to relax an interface between two immiscible liquids. Physical Chemistry Chemical Physics, 2011, 13, 13177.	2.8	27
61	Atomistic structure of amorphous silicon nitride from classical molecular dynamics simulations. Physical Review B, 2011, 83, .	3.2	33
62	Temperature accelerated Monte Carlo (TAMC): a method for sampling the free energy surface of non-analytical collective variables. Physical Chemistry Chemical Physics, 2011, 13, 5952.	2.8	31
63	Order-disorder phase change in embedded Si nanoparticles. Physical Review B, 2011, 83, .	3.2	8
64	Hydrodynamics from dynamical non-equilibrium MD. AIP Conference Proceedings, 2011, , .	0.4	5
65	Combining Rare Events Techniques: Phase Change in Si Nanoparticles. Journal of Statistical Physics, 2011, 145, 812-830.	1.2	12
66	Mechanisms of self-diffusion in stoichiometric and substoichiometric amorphous silicon dioxide. Physical Review B, 2010, 81, .	3.2	13
67	Modified single sweep method for reconstructing free-energy landscapes. Molecular Simulation, 2009, 35, 1116-1129.	2.0	13
68	Calculations of free energy barriers for local mechanisms of hydrogen diffusion in alanates. Scientific Modeling and Simulation SMNS, 2008, 15, 187-206.	0.8	21
69	Interface structure and defects of silicon nanocrystals embedded into a-SiO2. Applied Physics Letters, 2008, 93, 153109.	3.3	27
70	Calculations of free energy barriers for local mechanisms of hydrogen diffusion in alanates. Lecture Notes in Computational Science and Engineering, 2008, , 187-206.	0.3	3
71	STRUCTURAL AND ELECTRONIC PROPERTIES OF METAL-DOPED ORGANIC SEMICONDUCTORS. Modern Physics Letters B, 2008, 22, 1609-1631.	1.9	3
72	Dissociative versus molecular adsorption of phenol on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Si</mml:mi><mml:mrow><mml:mo>(</mml:mo><mml:mn>100</mml:mn><mml:mo>)</mml:mo></mml:mrow></mml:mrow> A first-principles calculation. Physical Review B, 2007, 76, .	3.2	19

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73	Quasi-One-Dimensional K-O Chain in PTCDA Thin Films: Evidence from First-Principles Calculations. Physical Review Letters, 2007, 98, 046401.	7.8	18
74	Efficient particle labeling in atomistic simulations. Journal of Chemical Physics, 2007, 126, 121102.	3.0	35
75	Ab Initio Simulation of Carbon Clustering on an Ni(111) Surface:Â A Model of the Poisoning of Nickel-Based Catalystsâ€. Journal of Physical Chemistry B, 2006, 110, 3638-3646.	2.6	44
76	Computational Materials Science application programming interface (CMSapi): a tool for developing applications for atomistic simulations. Computer Physics Communications, 2005, 169, 462-466.	7.5	9
77	Molecular and solid-state (8-hydroxy-quinoline)aluminum interaction with magnesium: A first-principles study. Journal of Applied Physics, 2005, 98, 023707.	2.5	15
78	Boron ripening in amorphous silicon by large scale molecular dynamics simulations. Computational Materials Science, 2004, 30, 143-149.	3.0	2
79	Energy-dispersive X-ray diffraction on thin films and its application to superconducting samples. Journal of Applied Crystallography, 2003, 36, 43-47.	4.5	3
80	Chemistry between Magnesium and Multiple Molecules in Tris(8-hydroxyquinoline) Aluminum Films. Journal of the American Chemical Society, 2003, 125, 7808-7809.	13.7	33
81	The monoclinic I2 structure of bassanite, calcium sulphate hemihydrate (CaSO4 0.5H2O). European Journal of Mineralogy, 2001, 13, 985-993.	1.3	78
82	SO2Cl2, SOCl2: energy dispersive X-ray diffraction, ab initio and molecular dynamics calculation. Computational Materials Science, 2001, 20, 407-415.	3.0	7
83	A novel implicit Newtonâ€“Raphson geometry optimization method for density functional theory calculations. Journal of Chemical Physics, 2001, 115, 636-642.	3.0	15
84	Low-energy electron scattering from the water molecule: Angular distributions and rotational excitation. Journal of Chemical Physics, 1998, 108, 4002-4012.	3.0	36