Simone Meloni

List of Publications by Year
in descending order

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84	4,342	172386	110317
papers	citations	29 h-index	64 g-index

91	91	91	6919
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Entropic stabilization of mixed A-cation ABX₃ metal halide perovskites for high performance perovskite solar cells. Energy and Environmental Science, 2016, 9, 656-662.	15.6	1,077
2	Ionic polarization-induced currentâ€“voltage hysteresis in CH3NH3PbX3 perovskite solar cells. Nature Communications, 2016, 7, 10334.	5.8	602
3	Origin of unusual bandgap shift and dual emission in organic-inorganic lead halide perovskites. Science Advances, 2016, 2, e1601156.	4.7	307
4	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.	1.6	179
5	Valence and conduction band tuning in halide perovskites for solar cell applications. Journal of Materials Chemistry A, 2016, 4, 15997-16002.	5.2	132
6	Metastable Wetting on Superhydrophobic Surfaces: Continuum and Atomistic Views of the Cassie-Baxterâ€“Wenzel Transition. Physical Review Letters, 2012, 109, 226102.	2.9	131
7	The Role of Grain Boundaries on Ionic Defect Migration in Metal Halide Perovskites. Advanced Energy Materials, 2020, 10, 1903735.	10.2	117
8	Methane Clathrate Hydrate Nucleation Mechanism by Advanced Molecular Simulations. Journal of Physical Chemistry C, 2014, 118, 22847-22857.	1.5	87
9	The monoclinic I2 structure of bassanite, calcium sulphate hemihydrate (CaSO4 0.5H2O). European Journal of Mineralogy, 2001, 13, 985-993.	0.4	78
10	Dual effect of humidity on cesium lead bromide: enhancement and degradation of perovskite films. Journal of Materials Chemistry A, 2019, 7, 12292-12302.	5.2	74
11	Collective Molecular Mechanisms in the CH₃NH₃PbI₃ Dissolution by Liquid Water. ACS Nano, 2017, 11, 9183-9190.	7.3	73
12	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.	5.2	57
13	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.	1.2	56
14	Geometry as a Catalyst: How Vapor Cavities Nucleate from Defects. Langmuir, 2013, 29, 14873-14884.	1.6	49
15	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.	1.2	44
16	Theory and methods for rare events. European Physical Journal B, 2012, 85, 1.	0.6	43
17	Hydrophilicity and Water Contact Angle on Methylammonium Lead Iodide. Advanced Materials Interfaces, 2019, 6, 1801173.	1.9	43
18	Accuracy of Molecular Simulation-Based Predictions of k_{off} Values: A Metadynamics Study. Journal of Physical Chemistry Letters, 2020, 11, 6373-6381.	2.1	41

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19	Unraveling the Salvinia Paradox: Design Principles for Submerged Superhydrophobicity. Advanced Materials Interfaces, 2015, 2, 1500248.	1.9	39
20	Computational Characterization of the Dependence of Halide Perovskite Effective Masses on Chemical Composition and Structure. Journal of Physical Chemistry C, 2017, 121, 23886-23895.	1.5	38
21	Focus Article: Theoretical aspects of vapor/gas nucleation at structured surfaces. Journal of Chemical Physics, 2016, 145, 211802.	1.2	37
22	Low-energy electron scattering from the water molecule: Angular distributions and rotational excitation. Journal of Chemical Physics, 1998, 108, 4002-4012.	1.2	36
23	Efficient particle labeling in atomistic simulations. Journal of Chemical Physics, 2007, 126, 121102.	1.2	35
24	Mechanism of the Cassie-Wenzel transition via the atomistic and continuum string methods. Journal of Chemical Physics, 2015, 142, 104701.	1.2	35
25	Chemistry between Magnesium and Multiple Molecules in Tris(8-hydroxyquinoline) Aluminum Films. Journal of the American Chemical Society, 2003, 125, 7808-7809.	6.6	33
26	Atomistic structure of amorphous silicon nitride from classical molecular dynamics simulations. Physical Review B, 2011, 83, .	1.1	33
27	Clathrate structure-type recognition: Application to hydrate nucleation and crystallisation. Journal of Chemical Physics, 2015, 142, 244503.	1.2	33
28	Extreme Scalability of DFT-Based QM/MM MD Simulations Using MiMiC. Journal of Chemical Theory and Computation, 2019, 15, 5601-5613.	2.3	32
29	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.	1.3	31
30	MiMiC: A Novel Framework for Multiscale Modeling in Computational Chemistry. Journal of Chemical Theory and Computation, 2019, 15, 3810-3823.	2.3	31
31	Mechanisms and Nucleation Rate of Methane Hydrate by Dynamical Nonequilibrium Molecular Dynamics. Journal of Physical Chemistry C, 2017, 121, 24223-24234.	1.5	30
32	Self-Recovery Superhydrophobic Surfaces: Modular Design. ACS Nano, 2018, 12, 359-367.	7.3	29
33	Crystalâ€Sizeâ€Induced Band Gap Tuning in Perovskite Films. Angewandte Chemie - International Edition, 2021, 60, 21368-21376.	7.2	28
34	Interface structure and defects of silicon nanocrystals embedded into a-SiO2. Applied Physics Letters, 2008, 93, 153109.	1.5	27
35	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.	1.3	27
36	The interplay among gas, liquid and solid interactions determines the stability of surface nanobubbles. Nanoscale, 2020, 12, 22698-22709.	2.8	27

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37	Pore Morphology Determines Spontaneous Liquid Extrusion from Nanopores. ACS Nano, 2019, 13, 1728-1738.	7.3	25
38	Atomistic Origins of the Limited Phase Stability of Cs⁺-Rich FA_xCs_(1â€“x)PbI₃ Mixtures. Chemistry of Materials, 2020, 32, 2605-2614.	3.2	24
39	Giant Negative Compressibility by Liquid Intrusion into Superhydrophobic Flexible Nanoporous Frameworks. Nano Letters, 2021, 21, 2848-2853.	4.5	24
40	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
41	Molecular Basis of CLC Antiporter Inhibition by Fluoride. Journal of the American Chemical Society, 2020, 142, 7254-7258.	6.6	20
42	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, .	1.1	19
43	Pressure control in interfacial systems: Atomistic simulations of vapor nucleation. Journal of Chemical Physics, 2018, 148, 064706.	1.2	19
44	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.	3.1	19
45	Collapse of superhydrophobicity on nanopillared surfaces. Physical Review Fluids, 2017, 2, .	1.0	19
46	Quasi-One-Dimensional K-O Chain in PTCDA Thin Films: Evidence from First-Principles Calculations. Physical Review Letters, 2007, 98, 046401.	2.9	18
47	Intrusion and extrusion of a liquid on nanostructured surfaces. Journal of Physics Condensed Matter, 2017, 29, 014003.	0.7	18
48	Liquid intrusion in and extrusion from non-wettable nanopores for technological applications. European Physical Journal B, 2021, 94, 1.	0.6	18
49	Probing the Structures of Hydrated Nafion in Different Morphologies Using Temperature-Accelerated Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2013, 117, 774-782.	1.5	17
50	A novel implicit Newtonâ€“Raphson geometry optimization method for density functional theory calculations. Journal of Chemical Physics, 2001, 115, 636-642.	1.2	15
51	Molecular and solid-state (8-hydroxy-quinoline)aluminum interaction with magnesium: A first-principles study. Journal of Applied Physics, 2005, 98, 023707.	1.1	15
52	Viscosity at the Nanoscale: Confined Liquid Dynamics and Thermal Effects in Self-Recovering Nanobumpers. Journal of Physical Chemistry C, 2018, 122, 14248-14256.	1.5	15
53	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
54	Wetting and recovery of nano-patterned surfaces beyond the classical picture. Nanoscale, 2019, 11, 21458-21470.	2.8	14

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55	Modified single sweep method for reconstructing free-energy landscapes. Molecular Simulation, 2009, 35, 1116-1129.	0.9	13
56	Mechanisms of self-diffusion in stoichiometric and substoichiometric amorphous silicon dioxide. Physical Review B, 2010, 81, .	1.1	13
57	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.	1.1	13
58	Combining Rare Events Techniques: Phase Change in Si Nanoparticles. Journal of Statistical Physics, 2011, 145, 812-830.	0.5	12
59	Kinetics and energeticsÂof metal halide perovskite conversion reactions at the nanoscale. Communications Materials, 2022, 3, .	2.9	12
60	The influence of silicon nanoclusters on the optical properties of a-SiNx samples: A theoretical study. Applied Physics Letters, 2012, 100, 181905.	1.5	11
61	Extended Intermolecular Interactions Governing Photocurrentâ€“Voltage Relations in Ternary Organic Solar Cells. Journal of Physical Chemistry Letters, 2016, 7, 3936-3944.	2.1	11
62	Activated Wetting of Nanostructured Surfaces: Reaction Coordinates, Finite Size Effects, and Simulation Pitfalls. Journal of Physical Chemistry B, 2018, 122, 200-212.	1.2	11
63	Subnanometer Topological Tuning of the Liquid Intrusion/Extrusion Characteristics of Hydrophobic Micropores. Nano Letters, 2022, 22, 2164-2169.	4.5	11
64	Relaxation of a steep density gradient in a simple fluid: Comparison between atomistic and continuum modeling. Journal of Chemical Physics, 2014, 141, 154107.	1.2	10
65	Free energies for rare events: Temperature accelerated MD and MC. European Physical Journal: Special Topics, 2015, 224, 2389-2407.	1.2	10
66	Defect Dynamics in MAPbI₃ Polycrystalline Films: The Trapping Effect of Grain Boundaries. Helvetica Chimica Acta, 2020, 103, e2000110.	1.0	10
67	Crystalâ€Sizeâ€Induced Band Gap Tuning in Perovskite Films. Angewandte Chemie, 2021, 133, 21538-21546.	1.6	10
68	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.	4.0	10
69	Computational Materials Science application programming interface (CMSapi): a tool for developing applications for atomistic simulations. Computer Physics Communications, 2005, 169, 462-466.	3.0	9
70	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.	1.5	9
71	Intrusion and extrusion of liquids in highly confining media: bridging fundamental research to applications. Advances in Physics: X, 2022, 7, .	1.5	9
72	Order-disorder phase change in embedded Si nanoparticles. Physical Review B, 2011, 83, .	1.1	8

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73	SO2Cl2, SOCl2: energy dispersive X-ray diffraction, ab initio and molecular dynamics calculation. Computational Materials Science, 2001, 20, 407-415.	1.4	7
74	Effect of the Topology on Wetting and Drying of Hydrophobic Porous Materials. ACS Applied Materials & Interfaces, 2022, 14, 30067-30079.	4.0	6
75	Hydrodynamics from dynamical non-equilibrium MD. AIP Conference Proceedings, 2011, , .	0.3	5
76	An observable for vacancy characterization and diffusion in crystals. Journal of Chemical Physics, 2013, 138, 144103.	1.2	5
77	MiMiC: Multiscale Modeling in Computational Chemistry. Frontiers in Molecular Biosciences, 2020, 7, 45.	1.6	5
78	Energy-dispersive X-ray diffraction on thin films and its application to superconducting samples. Journal of Applied Crystallography, 2003, 36, 43-47.	1.9	3
79	Calculations of free energy barriers for local mechanisms of hydrogen diffusion in alanates. Lecture Notes in Computational Science and Engineering, 2008, , 187-206.	0.1	3
80	STRUCTURAL AND ELECTRONIC PROPERTIES OF METAL-DOPED ORGANIC SEMICONDUCTORS. Modern Physics Letters B, 2008, 22, 1609-1631.	1.0	3
81	Boron ripening in amorphous silicon by large scale molecular dynamics simulations. Computational Materials Science, 2004, 30, 143-149.	1.4	2
82	Nucleation of silicon nanoparticles in amorphous silicon dioxide matrices. , 2014, , .		2
83	Wavefunction-Based Electrostatic-Embedding QM/MM Using CFOUR through MiMiC. Journal of Chemical Theory and Computation, 2022, 18, 13-24.	2.3	2
84	10.1063/1.4913839.5. , 2015, , .		0