Daniele Passerone

List of Publications by Year
in descending order

84 papers	5,421 citations	147801 31 h-index	79698 73 g-index
88 all docs	88 docs citations	88 times ranked	6963 citing authors

#	Article	IF	Citations
1	Asymmetric Elimination Reaction on Chiral Metal Surfaces. Advanced Materials, 2022, 34, e2104481.	21.0	9
2	On-surface synthesis and characterization of nitrogen-substituted undecacenes. Nature Communications, 2022, 13, 511.	12.8	26
3	Mapping the Structure of Oxygen-Doped Wurtzite Aluminum Nitride Coatings from Ab Initio Random Structure Search and Experiments. ACS Applied Materials & Interfaces, 2021, 13, 5762-5771.	8.0	3
4	AiiDAlab â€“ an ecosystem for developing, executing, and sharing scientific workflows. Computational Materials Science, 2021, 188, 110165.	3.0	40
5	Graphene nanoribbons with mixed cove-cape-zigzag edge structure. Carbon, 2021, 175, 50-59.	10.3	20
6	Metallic carbon nanotube quantum dots with broken symmetries as a platform for tunable terahertz detection. Applied Physics Reviews, 2021, 8, .	11.3	5
7	Robust, Multi-Length-Scale, Machine Learning Potential for Agâ€“Au Bimetallic Alloys from Clusters to Bulk Materials. Journal of Physical Chemistry C, 2021, 125, 17438-17447.	3.1	31
8	The Structure of Subâ€nm Platinum Clusters at Elevated Temperatures. Angewandte Chemie - International Edition, 2020, 59, 839-845.	13.8	29
9	The Structure of Subâ€nm Platinum Clusters at Elevated Temperatures. Angewandte Chemie, 2020, 132, 849-855.	2.0	7
10	Smart local orbitals for efficient calculations within density functional theory and beyond. Journal of Chemical Physics, 2020, 153, 194103.	3.0	8
11	Materials Cloud, a platform for open computational science. Scientific Data, 2020, 7, 299.	5.3	189
12	Atomic structure and electronic properties of planar defects in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>SrFe</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mrow><mml:mn>3</mml:mn><mml:mrow><mml:mtext>â˜’</mml:mtext><mml:mml>Î´</mml:m thin films. Physical Review Materials, 2020, 4, .	2.4	1
13	The reaction mechanism of the azideâ€“alkyne Huisgen cycloaddition. Physical Chemistry Chemical Physics, 2019, 21, 19281-19287.	2.8	8
14	Open-Shell Nonbenzenoid Nanographenes Containing Two Pairs of Pentagonal and Heptagonal Rings. Journal of the American Chemical Society, 2019, 141, 12011-12020.	13.7	112
15	Band Gap of Atomically Precise Graphene Nanoribbons as a Function of Ribbon Length and Termination. ChemPhysChem, 2019, 20, 2348-2353.	2.1	17
16	Template-Assisted in Situ Synthesis of Ag@Au Bimetallic Nanostructures Employing Liquid-Phase Transmission Electron Microscopy. ACS Nano, 2019, 13, 13333-13342.	14.6	32
17	Reliability of two embedded atom models for the description of Ag@Au nanoalloys. Journal of Chemical Physics, 2019, 151, 064105.	3.0	9
18	Overcoming Steric Hindrance in Arylâ€Aryl Homocoupling via Onâ€Surface Copolymerization. ChemPhysChem, 2019, 20, 2360-2366.	2.1	14

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19	Structure and properties of edge dislocations in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>BiFe</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review Materials, 2019, 3, .	2.4	7
20	Hidden Beneath the Surface: Origin of the Observed Enantioselective Adsorption on PdGa(111). Journal of the American Chemical Society, 2018, 140, 1401-1408.	13.7	16
21	Grown with the wind. Nature Materials, 2018, 17, 296-297.	27.5	0
22	Action spectra associated with inelastic two-electron tunneling through a single molecule: Propene on Cu(211). Surface Science, 2018, 678, 206-214.	1.9	3
23	Stair-rod dislocation cores acting as one-dimensional charge channels in GaAs nanowires. Physical Review Materials, 2018, 2, .	2.4	1
24	Stability of edge magnetism in functionalized zigzag graphene nanoribbons. Carbon, 2017, 124, 123-132.	10.3	21
25	Strain-driven oxygen deficiency in multiferroic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrMnO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> films. Physical Review B, 2016, 94, .	3.2	56
26	Water Formation for the Metalation of Porphyrin Molecules on Oxidized Cu(111). Chemistry - A European Journal, 2016, 22, 14672-14677.	3.3	18
27	Insight into structural phase transitions from the decoupled anharmonic mode approximation. Journal of Physics Condensed Matter, 2016, 28, 305401.	1.8	7
28	Silicon etch with chromium ions generated by a filtered or non-filtered cathodic arc discharge. Science and Technology of Advanced Materials, 2016, 17, 20-28.	6.1	1
29	Origin of distinct hydrogen absorption behavior of Zr2Pd and ZrPd2. International Journal of Hydrogen Energy, 2016, 41, 1736-1743.	7.1	4
30	On-surface synthesis of graphene nanoribbons with zigzag edge topology. Nature, 2016, 531, 489-492.	27.8	1,154
31	Synthesis of Atomically Precise Graphene-Based Nanostructures: A Simulation Point of View. Advances in Atom and Single Molecule Machines, 2016, , 237-268.	0.0	5
32	Superlubricity of graphene nanoribbons on gold surfaces. Science, 2016, 351, 957-961.	12.6	302
33	Direct Evidence of Surface Reduction in Monoclinic BiVO₄. Chemistry of Materials, 2015, 27, 3593-3600.	6.7	78
34	Role of interface coupling inhomogeneity in domain evolution in exchange bias. Scientific Reports, 2015, 4, 4508.	3.3	11
35	Microscale Motion Control through Ferromagnetic Films. Advanced Materials Interfaces, 2014, 1, 1400023.	3.7	5
36	Chiral reconstruction of Cu(110) after adsorption of fumaric acid. Surface Science, 2014, 629, 75-80.	1.9	8

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37	Surface layer evolution caused by the bombardment with ionized metal vapor. Nuclear Instruments & Methods in Physics Research B, 2014, 332, 337-340.	1.4	4
38	Identifying Photoreaction Products in Cinnamate-Based Photoalignment Materials. Journal of Physical Chemistry C, 2014, 118, 15422-15433.	3.1	4
39	Does rotational melting make molecular crystal surfaces more slippery?. Nanoscale, 2014, 6, 13163-13168.	5.6	3
40	Adsorption of Small Hydrocarbons on the Three-Fold PdGa Surfaces: The Road to Selective Hydrogenation. Journal of the American Chemical Society, 2014, 136, 11792-11798.	13.7	90
41	Ensemble Effect Evidenced by CO Adsorption on the 3-Fold PdGa Surfaces. Journal of Physical Chemistry C, 2014, 118, 12260-12265.	3.1	34
42	Real space crystallography of a complex metallic alloy: high-angle annular dark-field scanning transmission electron microscopy of o-Al₄(Cr,Fe). Journal of Applied Crystallography, 2014, 47, 1026-1031.	4.5	5
43	Chirality Transfer in 1D Self-Assemblies: Influence of H-Bonding vs Metal Coordination between Dicyano[7]helicene Enantiomers. Journal of the American Chemical Society, 2013, 135, 15270-15273.	13.7	57
44	Termini of Bottom-Up Fabricated Graphene Nanoribbons. Journal of the American Chemical Society, 2013, 135, 2060-2063.	13.7	214
45	Adsorption and Friction Behavior of Amphiphilic Polymers on Hydrophobic Surfaces. Langmuir, 2013, 29, 4760-4771.	3.5	8
46	Simulation of Adsorption Processes at Metallic Interfaces: An Image Charge Augmented QM/MM Approach. Journal of Chemical Theory and Computation, 2013, 9, 5086-5097.	5.3	65
47	Interface-confined mixing and buried partial dislocations for Ag bilayer on Pt(111). Physical Review B, 2012, 86, .	3.2	10
48	Phase constitution and interface structure of nano-sized Ag-Cu/AlN multilayers: Experiment and ab initio modeling. Applied Physics Letters, 2012, 101, .	3.3	16
49	Room Temperature Metalation of 2H-TPP Monolayer on Iron and Nickel Surfaces by Picking up Substrate Metal Atoms. ACS Nano, 2012, 6, 10800-10807.	14.6	63
50	Intraribbon Heterojunction Formation in Ultranarrow Graphene Nanoribbons. ACS Nano, 2012, 6, 2020-2025.	14.6	169
51	An ab initio insight into the Cu(111)-mediated Ullmann reaction. Physical Chemistry Chemical Physics, 2011, 13, 154-160.	2.8	75
52	Two-Dimensional Self-Assembly of Chiral Malic Acid on Cu(110). Journal of Physical Chemistry C, 2011, 115, 1240-1247.	3.1	24
53	Surface-assisted cyclodehydrogenation provides a synthetic route towards easily processable and chemically tailored nanographenes. Nature Chemistry, 2011, 3, 61-67.	13.6	395
54	Selfâ€Assembly and Twoâ€Dimensional Spontaneous Resolution of Cyanoâ€Functionalized [7]Helicenes on Cu(111). Angewandte Chemie - International Edition, 2011, 50, 9982-9986.	13.8	94

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55	Supramolecular Engineering through Temperatureâ€Induced Chemical Modification of 2Hâ€Tetraphenylporphyrin on Ag(111): Flat Phenyl Conformation and Possible Dehydrogenation Reactions. Chemistry - A European Journal, 2011, 17, 14354-14359.	3.3	58
56	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>s</mml:mi></mml:math>-orbital continuum model accounting for the tip shape in simulated scanning tunneling microscope images. Physical Review B, 2011, 84, .	3.2	8
57	A simple approach for describing metal-supported cyclohexaphenylene dehydrogenation. European Physical Journal B, 2010, 75, 65-70.	1.5	11
58	Ab initio simulations of the Ag(111)/Al2O3 interface at intermediate oxygen partial pressures. Journal of Materials Science, 2010, 45, 4265-4270.	3.7	14
59	Porous Graphene as an Atmospheric Nanofilter. Small, 2010, 6, 2266-2271.	10.0	325
60	Atomistic insight into the adsorption site selectivity of stepped Au(111) surfaces. Physical Review B, 2010, 82, .	3.2	17
61	Two-Dimensional Polymer Formation on Surfaces: Insight into the Roles of Precursor Mobility and Reactivity. Journal of the American Chemical Society, 2010, 132, 16669-16676.	13.7	449
62	Probing the selectivity of a nanostructured surface by xenon adsorption. Nanoscale, 2010, 2, 502.	5.6	25
63	The role of van der Waals interactions in surface-supported supramolecular networks. Physical Chemistry Chemical Physics, 2010, 12, 992-999.	2.8	44
64	Switching the Chirality of Single Adsorbate Complexes. Angewandte Chemie - International Edition, 2009, 48, 4065-4068.	13.8	96
65	Tailoring Low-Dimensional Organic Semiconductor Nanostructures. Nano Letters, 2009, 9, 126-131.	9.1	33
66	Tonelli Principle: Finite Reduction and Fixed Energy Molecular Dynamics Trajectories. Multiscale Modeling and Simulation, 2009, 7, 1171-1191.	1.6	2
67	Oxygen influence on ceramics wettability by liquid metals: Ag/Î±-Al2O3â€”Experiments and modelling. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2008, 495, 153-158.	5.6	36
68	Modeling bulk and surface Pt using the â€œGaussian and plane waveâ€•density functional theory formalism: Validation and comparison to k-point plane wave calculations. Journal of Chemical Physics, 2008, 129, 234703.	3.0	36
69	C₆₀/Corannulene on Cu(110):â€‰ A Surface-Supported Bistable Buckybowlâ^'Buckyball Hostâ^'Guest System. Journal of the American Chemical Society, 2008, 130, 4767-4771.	13.7	109
70	Liquid metal/ceramic interactions in the (Cu, Ag, Au)/ZrB2 systems. Journal of the European Ceramic Society, 2007, 27, 3277-3285.	5.7	56
71	Wetting of Group IV diborides by liquid metals. Journal of Materials Science, 2006, 41, 5088-5098.	3.7	45
72	Computing the density of paths in complex systems. Journal of Chemical Physics, 2006, 124, 134103.	3.0	3

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73	The Microscopic Switching Mechanism of a [2]Catenane. Journal of Physical Chemistry B, 2005, 109, 17094-17099.	2.6	27
74	Solidification of Gold Nanoparticles in Carbon Nanotubes. Physical Review Letters, 2005, 94, 105502.	7.8	111
75	Exploring conical intersection spaces using pseudo-dynamics and band optimization: a novel strategy. Computer Physics Communications, 2005, 169, 305-308.	7.5	2
76	Pseudo-dynamics and band optimizations: shedding light into conical intersection seams. Chemical Physics Letters, 2004, 389, 1-6.	2.6	21
77	Insights into the Electronic Dynamics in Chemical Reactions. Journal of Physical Chemistry A, 2004, 108, 848-854.	2.5	17
78	A concerted variational strategy for investigating rare events. Journal of Chemical Physics, 2003, 118, 2025-2032.	3.0	61
79	Action-Derived Molecular Dynamics in the Study of Rare Events. Physical Review Letters, 2001, 87, 108302.	7.8	134
80	(Meta)stable reconstructions of the diamond (111) surface: Interplay between diamond and graphitelike bonding. Physical Review B, 2000, 61, R10590-R10593.	3.2	20
81	Reentrant Layering in Rare Gas Adsorption: Preroughening or Premelting?. Physical Review Letters, 2000, 84, 2203-2206.	7.8	12
82	Variable-curvature-slab molecular dynamics as a method to determine surface stress. Physical Review B, 1999, 59, 7687-7696.	3.2	15
83	Reconstruction of Diamond (001) Surface: A Monte Carlo Study with the Tersoff Potential. Physica Status Solidi A, 1999, 174, 19-23.	1.7	8
84	Atom-surface scattering from palladium growth clusters. Surface Science, 1995, 342, 307-318.	1.9	2