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	On-surface synthesis of graphene nanoribbons with zigzag edge topology. Nature, 2016, 531, 489-492.	27.8	1,154
2	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
3	Surface-assisted cyclodehydrogenation provides a synthetic route towards easily processable and chemically tailored nanographenes. Nature Chemistry, 2011, 3, 61-67.	13.6	395
4	Porous Graphene as an Atmospheric Nanofilter. Small, 2010, 6, 2266-2271.	10.0	325
5	Superlubricity of graphene nanoribbons on gold surfaces. Science, 2016, 351, 957-961.	12.6	302
6	Termini of Bottom-Up Fabricated Graphene Nanoribbons. Journal of the American Chemical Society, 2013, 135, 2060-2063.	13.7	214
7	Materials Cloud, a platform for open computational science. Scientific Data, 2020, 7, 299.	5.3	189
8	Intraribbon Heterojunction Formation in Ultranarrow Graphene Nanoribbons. ACS Nano, 2012, 6, 2020-2025.	14.6	169
9	Action-Derived Molecular Dynamics in the Study of Rare Events. Physical Review Letters, 2001, 87, 108302.	7.8	134
10	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
11	Solidification of Gold Nanoparticles in Carbon Nanotubes. Physical Review Letters, 2005, 94, 105502.	7.8	111
12	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
13	Switching the Chirality of Single Adsorbate Complexes. Angewandte Chemie - International Edition, 2009, 48, 4065-4068.	13.8	96
14	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
15	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
16	Direct Evidence of Surface Reduction in Monoclinic BiVO₄. Chemistry of Materials, 2015, 27, 3593-3600.	6.7	78
17	An ab initio insight into the Cu(111)-mediated Ullmann reaction. Physical Chemistry Chemical Physics, 2011, 13, 154-160.	2.8	75
18	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

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19	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
20	A concerted variational strategy for investigating rare events. Journal of Chemical Physics, 2003, 118, 2025-2032.	3.0	61
21	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
22	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
23	Liquid metal/ceramic interactions in the (Cu, Ag, Au)/ZrB2 systems. Journal of the European Ceramic Society, 2007, 27, 3277-3285.	5.7	56
24	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></ films. Physical Review B, 2016, 94, .	3.2	56
25	Wetting of Group IV diborides by liquid metals. Journal of Materials Science, 2006, 41, 5088-5098.	3.7	45
26	The role of van der Waals interactions in surface-supported supramolecular networks. Physical Chemistry Chemical Physics, 2010, 12, 992-999.	2.8	44
27	AiiDAlab â€“ an ecosystem for developing, executing, and sharing scientific workflows. Computational Materials Science, 2021, 188, 110165.	3.0	40
28	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
29	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
30	Ensemble Effect Evidenced by CO Adsorption on the 3-Fold PdGa Surfaces. Journal of Physical Chemistry C, 2014, 118, 12260-12265.	3.1	34
31	Tailoring Low-Dimensional Organic Semiconductor Nanostructures. Nano Letters, 2009, 9, 126-131.	9.1	33
32	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
33	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
34	The Structure of Subâ€nm Platinum Clusters at Elevated Temperatures. Angewandte Chemie - International Edition, 2020, 59, 839-845.	13.8	29
35	The Microscopic Switching Mechanism of a [2]Catenane. Journal of Physical Chemistry B, 2005, 109, 17094-17099.	2.6	27
36	On-surface synthesis and characterization of nitrogen-substituted undecacenes. Nature Communications, 2022, 13, 511.	12.8	26

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37	Probing the selectivity of a nanostructured surface by xenon adsorption. Nanoscale, 2010, 2, 502.	5.6	25
38	Two-Dimensional Self-Assembly of Chiral Malic Acid on Cu(110). Journal of Physical Chemistry C, 2011, 115, 1240-1247.	3.1	24
39	Pseudo-dynamics and band optimizations: shedding light into conical intersection seams. Chemical Physics Letters, 2004, 389, 1-6.	2.6	21
40	Stability of edge magnetism in functionalized zigzag graphene nanoribbons. Carbon, 2017, 124, 123-132.	10.3	21
41	(Meta)stable reconstructions of the diamond (111) surface: Interplay between diamond and graphitelike bonding. Physical Review B, 2000, 61, R10590-R10593.	3.2	20
42	Graphene nanoribbons with mixed cove-cape-zigzag edge structure. Carbon, 2021, 175, 50-59.	10.3	20
43	Water Formation for the Metalation of Porphyrin Molecules on Oxidized Cu(111). Chemistry - A European Journal, 2016, 22, 14672-14677.	3.3	18
44	Insights into the Electronic Dynamics in Chemical Reactions. Journal of Physical Chemistry A, 2004, 108, 848-854.	2.5	17
45	Atomistic insight into the adsorption site selectivity of stepped Au(111) surfaces. Physical Review B, 2010, 82, .	3.2	17
46	Band Gap of Atomically Precise Graphene Nanoribbons as a Function of Ribbon Length and Termination. ChemPhysChem, 2019, 20, 2348-2353.	2.1	17
47	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
48	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
49	Variable-curvature-slab molecular dynamics as a method to determine surface stress. Physical Review B, 1999, 59, 7687-7696.	3.2	15
50	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
51	Overcoming Steric Hindrance in Arylâ€Aryl Homocoupling via Onâ€Surface Copolymerization. ChemPhysChem, 2019, 20, 2360-2366.	2.1	14
52	Reentrant Layering in Rare Gas Adsorption: Preroughening or Premelting?. Physical Review Letters, 2000, 84, 2203-2206.	7.8	12
53	A simple approach for describing metal-supported cyclohexaphenylene dehydrogenation. European Physical Journal B, 2010, 75, 65-70.	1.5	11
54	Role of interface coupling inhomogeneity in domain evolution in exchange bias. Scientific Reports, 2015, 4, 4508.	3.3	11

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55	Interface-confined mixing and buried partial dislocations for Ag bilayer on Pt(111). Physical Review B, 2012, 86, .	3.2	10
56	Reliability of two embedded atom models for the description of Ag@Au nanoalloys. Journal of Chemical Physics, 2019, 151, 064105.	3.0	9
57	Asymmetric Elimination Reaction on Chiral Metal Surfaces. Advanced Materials, 2022, 34, e2104481.	21.0	9
58	Reconstruction of Diamond (001) Surface: A Monte Carlo Study with the Tersoff Potential. Physica Status Solidi A, 1999, 174, 19-23.	1.7	8
59	<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
60	Adsorption and Friction Behavior of Amphiphilic Polymers on Hydrophobic Surfaces. Langmuir, 2013, 29, 4760-4771.	3.5	8
61	Chiral reconstruction of Cu(110) after adsorption of fumaric acid. Surface Science, 2014, 629, 75-80.	1.9	8
62	The reaction mechanism of the azideâ€“alkyne Huisgen cycloaddition. Physical Chemistry Chemical Physics, 2019, 21, 19281-19287.	2.8	8
63	Smart local orbitals for efficient calculations within density functional theory and beyond. Journal of Chemical Physics, 2020, 153, 194103.	3.0	8
64	Insight into structural phase transitions from the decoupled anharmonic mode approximation. Journal of Physics Condensed Matter, 2016, 28, 305401.	1.8	7
65	The Structure of Subâ€nm Platinum Clusters at Elevated Temperatures. Angewandte Chemie, 2020, 132, 849-855.	2.0	7
66	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
67	Microscale Motion Control through Ferromagnetic Films. Advanced Materials Interfaces, 2014, 1, 1400023.	3.7	5
68	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
69	Metallic carbon nanotube quantum dots with broken symmetries as a platform for tunable terahertz detection. Applied Physics Reviews, 2021, 8, .	11.3	5
70	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
71	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
72	Identifying Photoreaction Products in Cinnamate-Based Photoalignment Materials. Journal of Physical Chemistry C, 2014, 118, 15422-15433.	3.1	4

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73	Origin of distinct hydrogen absorption behavior of Zr2Pd and ZrPd2. International Journal of Hydrogen Energy, 2016, 41, 1736-1743.	7.1	4
74	Computing the density of paths in complex systems. Journal of Chemical Physics, 2006, 124, 134103.	3.0	3
75	Does rotational melting make molecular crystal surfaces more slippery?. Nanoscale, 2014, 6, 13163-13168.	5.6	3
76	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
77	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
78	Atom-surface scattering from palladium growth clusters. Surface Science, 1995, 342, 307-318.	1.9	2
79	Exploring conical intersection spaces using pseudo-dynamics and band optimization: a novel strategy. Computer Physics Communications, 2005, 169, 305-308.	7.5	2
80	Tonelli Principle: Finite Reduction and Fixed Energy Molecular Dynamics Trajectories. Multiscale Modeling and Simulation, 2009, 7, 1171-1191.	1.6	2
81	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
82	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:ml>Î´</mml:m thin films. Physical Review Materials, 2020, 4, .	2.4	1
83	Stair-rod dislocation cores acting as one-dimensional charge channels in GaAs nanowires. Physical Review Materials, 2018, 2, .	2.4	1
84	Grown with the wind. Nature Materials, 2018, 17, 296-297.	27.5	0