Shobhana Narasimhan

List of Publications by Year
in descending order

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63	585	623734	642732
papers	citations	14 h-index	23 g-index

70	70	70	997
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Blue and black phosphorene on metal substrates: a density functional theory study. Journal of Physics Condensed Matter, 2022, 34, 084001.	1.8	1
2	Intersections 6: A (mostly) Scientific Crossword. Resonance, 2022, 27, 153-155.	0.3	0
3	Intersections 5: A (mostly) Scientific Crossword. Resonance, 2022, 27, 157-157.	0.3	0
4	Intersections 7: A (mostly) Scientific Crossword. Resonance, 2022, 27, 297-299.	0.3	0
5	Intersections 6: A (mostly) Scientific Crossword. Resonance, 2022, 27, 301-301.	0.3	0
6	Intersections 7: A (mostly) Scientific Crossword. Resonance - Journal of Science Education, 2022, 27, 493-493.	0.3	0
7	Intersections 8: A (mostly) Scientific Crossword. Resonance - Journal of Science Education, 2022, 27, 490-492.	0.3	0
8	Intersections 8: A (mostly) Scientific Crossword. Resonance - Journal of Science Education, 2022, 27, 699-699.	0.3	0
9	Intersections 9: A (mostly) Scientific Crossword. Resonance - Journal of Science Education, 2022, 27, 696-698.	0.3	0
10	Intersections 9: A (mostly) Scientific Crossword. Resonance - Journal of Science Education, 2022, 27, 891-891.	0.3	0
11	Intersections 10: A (mostly) Scientific Crossword. Resonance - Journal of Science Education, 2022, 27, 892-894.	0.3	0
12	Identification and Manipulation of Defects in Black Phosphorus. Journal of Physical Chemistry Letters, 2022, 13, 6276-6282.	4.6	1
13	Leveraging Polar Discontinuities to Tune the Binding of Methanol on BCN and Grapheneâ€“BN Lateral Heterostructures. Journal of Physical Chemistry C, 2021, 125, 15012-15024.	3.1	5
14	Intersections 1: A (mostly) Scientific Crossword. Resonance, 2021, 26, 1175-1177.	0.3	0
15	Rotation in an Enantiospecific Selfâ€Assembled Array of Molecular Raffle Wheels. Angewandte Chemie - International Edition, 2021, 60, 26932-26938.	13.8	5
16	Intersections 1: A (mostly) Scientific Crossword. Resonance, 2021, 26, 1319-1319.	0.3	0
17	Intersections 2: A (mostly) Scientific Crossword. Resonance, 2021, 26, 1315-1317.	0.3	0
18	Intersections 4: A (mostly) Scientific Crossword. Resonance, 2021, 26, 1595-1597.	0.3	0

#	Article	IF	Citations
19	Intersections 3: A (mostly) Scientific Crossword. Resonance, 2021, 26, 1599-1599.	0.3	0
20	Intersections 4: A (mostly) Scientific Crossword. Resonance, 2021, 26, 1735-1735.	0.3	0
21	Intersections 5: A (mostly) Scientific Crossword. Resonance, 2021, 26, 1731-1733.	0.3	0
22	Harvesting Delayed Fluorescence in Perovskite Nanocrystals Using Spin-Forbidden Mn d States. ACS Energy Letters, 2020, 5, 353-359.	17.4	18
23	Direct Observation of the Reduction of a Molecule on Nitrogen Pairs in Doped Graphene. Nano Letters, 2020, 20, 6908-6913.	9.1	8
24	Enhanced hydrogen evolution reactivity on $${mathrm{Mo}}_2{mathrm{C}}$$â€“$${mathrm{Mo}}_2{mathrm{N}}$$ composites. Bulletin of Materials Science, 2020, 43, 1.	1.7	4
25	Cooperative particle rearrangements facilitate the self-organized growth of colloidal crystal arrays on strain-relief patterns. Science Advances, 2020, 6, eaay8418.	10.3	11
26	Support work function as a descriptor and predictor for the charge and morphology of deposited Au nanoparticles. Journal of Chemical Physics, 2020, 152, 144704.	3.0	3
27	A handle on the scandal: Data driven approaches to structure prediction. APL Materials, 2020, 8, 040903.	5.1	4
28	Adsorption of methane on single metal atoms supported on graphene: Role of electron back-donation in binding and activation. Journal of Chemical Physics, 2020, 153, 244701.	3.0	8
29	Descriptor for the Efficacy of Aliovalent Doping of Oxides and Its Application for the Charging of Supported Au Clusters. Journal of Physical Chemistry C, 2019, 123, 19794-19805.	3.1	4
30	A simple descriptor for binding and charge transfer at blue phosphorene-metal interfaces. Applied Surface Science, 2019, 492, 16-22.	6.1	5
31	Importance of Epitaxial Strain at a Spin-Crossover Moleculeâ€“Metal Interface. Journal of Physical Chemistry Letters, 2019, 10, 4103-4109.	4.6	39
32	Diffusion barriers, growth pathways, and scaling relations for small supported metal clusters. Journal of Chemical Physics, 2019, 151, 144709.	3.0	2
33	Selective control of molecule charge state on graphene using tip-induced electric field and nitrogen doping. Npj 2D Materials and Applications, 2019, 3, .	7.9	19
34	Using first principles calculations to interpret XANES experiments: extracting the size-dependence of the (pâ€Š, T) phase diagram of sub-nanometer Cu clusters in an O₂ environment. Journal of Physics Condensed Matter, 2019, 31, 144002.	1.8	6
35	Reversing Sizeâ€Dependent Trends in the Oxidation of Copper Clusters through Support Effects. European Journal of Inorganic Chemistry, 2018, 2018, 16-22.	2.0	20
36	Cover Feature: Reversing Size-Dependent Trends in the Oxidation of Copper Clusters through Support Effects (Eur. J. Inorg. Chem. 1/2018). European Journal of Inorganic Chemistry, 2018, 2018, 3-3.	2.0	0

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37	Inducing wetting morphologies and increased reactivities of small Au clusters on doped oxide supports. Journal of Chemical Physics, 2018, 149, 174701.	3.0	6
38	Descriptor-Based Rational Design of Two-Dimensional Self-Assembled Nanoarchitectures Stabilized by Hydrogen Bonds. Chemistry of Materials, 2017, 29, 7170-7182.	6.7	18
39	A tryst with density. Resonance, 2017, 22, 731-746.	0.3	0
40	Hum Kohn Hai. Resonance, 2017, 22, 725-729.	0.3	0
41	Graphene oxide as an optimal candidate material for methane storage. Journal of Chemical Physics, 2015, 143, 044704.	3.0	13
42	Substrate doping: A strategy for enhancing reactivity on gold nanocatalysts by tuning sp bands. Journal of Chemical Physics, 2015, 143, 144307.	3.0	9
43	Physical origins of weak H2 binding on carbon nanostructures: Insight from ab initio studies of chemically functionalized graphene nanoribbons. Journal of Chemical Physics, 2014, 140, 174708.	3.0	15
44	Enhanced Gas Adsorption on Graphitic Substrates via Defects and Local Curvature: A Density Functional Theory Study. Journal of Physical Chemistry C, 2014, 118, 7741-7750.	3.1	43
45	Ab initioand cluster expansion study of surface alloys of Fe and Au on Ru(0001) and Mo(110): Importance of magnetism. Physical Review B, 2013, 88, .	3.2	4
46	Tuning patterning conditions by co-adsorption of gases: Br2 and H2 on Si(001). Journal of Chemical Physics, 2013, 139, 184713.	3.0	3
47	Trends in the Electronic Structure of Extended Gold Compounds: Implications for Use of Gold in Heterogeneous Catalysis. Inorganic Chemistry, 2012, 51, 7569-7578.	4.0	7
48	Methane and carbon dioxide adsorption on edge-functionalized graphene: A comparative DFT study. Journal of Chemical Physics, 2012, 137, 054702.	3.0	105
49	Tuning the Morphology of Gold Clusters by Substrate Doping. Journal of the American Chemical Society, 2011, 133, 2801-2803.	13.7	56
50	Magnetism of surface alloys of the type MxN1â^'x/Rh(111). Journal of Magnetism and Magnetic Materials, 2011, 323, 1873-1881.	2.3	1
51	Prediction of reconstruction in heteroepitaxial systems using the Frenkel-Kontorova model. Physical Review B, 2011, 84, .	3.2	5
52	Ordered Surface Alloy of Bulk-Immiscible Components Stabilized by Magnetism. Physical Review Letters, 2010, 105, 056101.	7.8	21
53	Harmonic and anharmonic properties of Fe and Ni: Thermal expansion, exchange-correlation errors, and magnetism. Physical Review B, 2010, 82, .	3.2	19
54	Mixing and magnetic properties of surface alloys: The role of the substrate. Applied Surface Science, 2009, 256, 449-454.	6.1	2

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55	: A stable surface alloy with enhanced magnetic moments. Solid State Communications, 2009, 149, 559-563.	1.9	2
56	Elastic and chemical contributions to the stability of magnetic surface alloys on Ru(0001). Physical Review B, 2009, 79, .	3.2	12
57	Effect of coordination on bond properties: A first principles study. Bulletin of Materials Science, 2008, 31, 569-572.	1.7	9
58	Competition between elastic and chemical effects in the intermixing of Co and Ag on Rh(111). Journal of Chemical Sciences, 2008, 120, 621-626.	1.5	3
59	Bond stiffening in small nanoclusters and its consequences for mechanical and thermal properties. Physical Review B, 2008, 77, .	3.2	15
60	Symmetries, vibrational instabilities, and routes to stable structures of clusters of Al, Sn, and As. Journal of Chemical Physics, 2004, 121, 5211-5220.	3.0	21
61	Ab initio lattice dynamics of Ag(). Surface Science, 2002, 496, 331-344.	1.9	13
62	Ab initio calculations on the anomalous thermal behaviour of fcc(1 1 0) surfaces. Applied Surface Science, 2001, 182, 293-296.	6.1	5
63	Reversed anisotropies and thermal contraction of fcc (110) surfaces. Physical Review B, 2001, 64, .	3.2	15