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	Methane and carbon dioxide adsorption on edge-functionalized graphene: A comparative DFT study. Journal of Chemical Physics, 2012, 137, 054702.	3.0	105
2	Tuning the Morphology of Gold Clusters by Substrate Doping. Journal of the American Chemical Society, 2011, 133, 2801-2803.	13.7	56
3	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
4	Importance of Epitaxial Strain at a Spin-Crossover Moleculeâ€“Metal Interface. Journal of Physical Chemistry Letters, 2019, 10, 4103-4109.	4.6	39
5	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
6	Ordered Surface Alloy of Bulk-Immiscible Components Stabilized by Magnetism. Physical Review Letters, 2010, 105, 056101.	7.8	21
7	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
8	Harmonic and anharmonic properties of Fe and Ni: Thermal expansion, exchange-correlation errors, and magnetism. Physical Review B, 2010, 82, .	3.2	19
9	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
10	Descriptor-Based Rational Design of Two-Dimensional Self-Assembled Nanoarchitectures Stabilized by Hydrogen Bonds. Chemistry of Materials, 2017, 29, 7170-7182.	6.7	18
11	Harvesting Delayed Fluorescence in Perovskite Nanocrystals Using Spin-Forbidden Mn d States. ACS Energy Letters, 2020, 5, 353-359.	17.4	18
12	Reversed anisotropies and thermal contraction of fcc (110) surfaces. Physical Review B, 2001, 64, .	3.2	15
13	Bond stiffening in small nanoclusters and its consequences for mechanical and thermal properties. Physical Review B, 2008, 77, .	3.2	15
14	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
15	Ab initio lattice dynamics of Ag(). Surface Science, 2002, 496, 331-344.	1.9	13
16	Graphene oxide as an optimal candidate material for methane storage. Journal of Chemical Physics, 2015, 143, 044704.	3.0	13
17	Elastic and chemical contributions to the stability of magnetic surface alloys on Ru(0001). Physical Review B, 2009, 79, .	3.2	12
18	Cooperative particle rearrangements facilitate the self-organized growth of colloidal crystal arrays on strain-relief patterns. Science Advances, 2020, 6, eaay8418.	10.3	11

#	Article	IF	Citations
19	Effect of coordination on bond properties: A first principles study. Bulletin of Materials Science, 2008, 31, 569-572.	1.7	9
20	Substrate doping: A strategy for enhancing reactivity on gold nanocatalysts by tuning sp bands. Journal of Chemical Physics, 2015, 143, 144307.	3.0	9
21	Direct Observation of the Reduction of a Molecule on Nitrogen Pairs in Doped Graphene. Nano Letters, 2020, 20, 6908-6913.	9.1	8
22	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
23	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
24	Inducing wetting morphologies and increased reactivities of small Au clusters on doped oxide supports. Journal of Chemical Physics, 2018, 149, 174701.	3.0	6
25	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
26	Ab initio calculations on the anomalous thermal behaviour of fcc(1 1 0) surfaces. Applied Surface Science, 2001, 182, 293-296.	6.1	5
27	Prediction of reconstruction in heteroepitaxial systems using the Frenkel-Kontorova model. Physical Review B, 2011, 84, .	3.2	5
28	A simple descriptor for binding and charge transfer at blue phosphorene-metal interfaces. Applied Surface Science, 2019, 492, 16-22.	6.1	5
29	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
30	Rotation in an Enantiospecific Selfâ€Assembled Array of Molecular Raffle Wheels. Angewandte Chemie - International Edition, 2021, 60, 26932-26938.	13.8	5
31	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
32	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
33	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
34	A handle on the scandal: Data driven approaches to structure prediction. APL Materials, 2020, 8, 040903.	5.1	4
35	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
36	Tuning patterning conditions by co-adsorption of gases: Br2 and H2 on Si(001). Journal of Chemical Physics, 2013, 139, 184713.	3.0	3

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37	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
38	Mixing and magnetic properties of surface alloys: The role of the substrate. Applied Surface Science, 2009, 256, 449-454.	6.1	2
39	: A stable surface alloy with enhanced magnetic moments. Solid State Communications, 2009, 149, 559-563.	1.9	2
40	Diffusion barriers, growth pathways, and scaling relations for small supported metal clusters. Journal of Chemical Physics, 2019, 151, 144709.	3.0	2
41	Magnetism of surface alloys of the type MxN1â^'x/Rh(111). Journal of Magnetism and Magnetic Materials, 2011, 323, 1873-1881.	2.3	1
42	Blue and black phosphorene on metal substrates: a density functional theory study. Journal of Physics Condensed Matter, 2022, 34, 084001.	1.8	1
43	Identification and Manipulation of Defects in Black Phosphorus. Journal of Physical Chemistry Letters, 2022, 13, 6276-6282.	4.6	1
44	A tryst with density. Resonance, 2017, 22, 731-746.	0.3	0
45	Hum Kohn Hai. Resonance, 2017, 22, 725-729.	0.3	0
46	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
47	Intersections 1: A (mostly) Scientific Crossword. Resonance, 2021, 26, 1175-1177.	0.3	0
48	Intersections 1: A (mostly) Scientific Crossword. Resonance, 2021, 26, 1319-1319.	0.3	0
49	Intersections 2: A (mostly) Scientific Crossword. Resonance, 2021, 26, 1315-1317.	0.3	0
50	Intersections 4: A (mostly) Scientific Crossword. Resonance, 2021, 26, 1595-1597.	0.3	0
51	Intersections 6: A (mostly) Scientific Crossword. Resonance, 2022, 27, 153-155.	0.3	0
52	Intersections 5: A (mostly) Scientific Crossword. Resonance, 2022, 27, 157-157.	0.3	0
53	Intersections 7: A (mostly) Scientific Crossword. Resonance, 2022, 27, 297-299.	0.3	0
54	Intersections 6: A (mostly) Scientific Crossword. Resonance, 2022, 27, 301-301.	0.3	0

#	Article	IF	Citations
55	Intersections 7: A (mostly) Scientific Crossword. Resonance - Journal of Science Education, 2022, 27, 493-493.	0.3	0
56	Intersections 8: A (mostly) Scientific Crossword. Resonance - Journal of Science Education, 2022, 27, 490-492.	0.3	0
57	Intersections 3: A (mostly) Scientific Crossword. Resonance, 2021, 26, 1599-1599.	0.3	0
58	Intersections 4: A (mostly) Scientific Crossword. Resonance, 2021, 26, 1735-1735.	0.3	0
59	Intersections 5: A (mostly) Scientific Crossword. Resonance, 2021, 26, 1731-1733.	0.3	0
60	Intersections 8: A (mostly) Scientific Crossword. Resonance - Journal of Science Education, 2022, 27, 699-699.	0.3	0
61	Intersections 9: A (mostly) Scientific Crossword. Resonance - Journal of Science Education, 2022, 27, 696-698.	0.3	0
62	Intersections 9: A (mostly) Scientific Crossword. Resonance - Journal of Science Education, 2022, 27, 891-891.	0.3	0
63	Intersections 10: A (mostly) Scientific Crossword. Resonance - Journal of Science Education, 2022, 27, 892-894.	0.3	0