Ashwin Ramasubramaniam

List of Publications by Year
in descending order

83 papers	8,243 citations	117625 34 h-index	56724 83 g-index
86 all docs	86 docs citations	86 times ranked	13093 citing authors

#	Article	IF	Citations
1	Two-dimensional material nanophotonics. Nature Photonics, 2014, 8, 899-907.	31.4	2,362
2	Large excitonic effects in monolayers of molybdenum and tungsten dichalcogenides. Physical Review B, 2012, 86, .	3.2	1,250
3	Hydrogen Bond Networks in Graphene Oxide Composite Paper: Structure and Mechanical Properties. ACS Nano, 2010, 4, 2300-2306.	14.6	674
4	Tunable band gaps in bilayer transition-metal dichalcogenides. Physical Review B, 2011, 84, .	3.2	538
5	Mn-doped monolayer MoS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>: An atomically thin dilute magnetic semiconductor. Physical Review B, 2013, 87, .	3.2	413
6	Edge-Stress-Induced Warping of Graphene Sheets and Nanoribbons. Physical Review Letters, 2008, 101, 245501.	7.8	321
7	Tunable Band Gaps in Bilayer Grapheneâ^'BN Heterostructures. Nano Letters, 2011, 11, 1070-1075.	9.1	224
8	Binding of Pt Nanoclusters to Point Defects in Graphene: Adsorption, Morphology, and Electronic Structure. Journal of Physical Chemistry C, 2012, 116, 6543-6555.	3.1	224
9	Interatomic potentials for hydrogen in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>â€“iron based on density functional theory. Physical Review B, 2009, 79, .	3.2	166
10	Ab initiostudies of thermodynamic and electronic properties of phosphorene nanoribbons. Physical Review B, 2014, 90, .	3.2	126
11	Edge elastic properties of defect-free single-layer graphene sheets. Applied Physics Letters, 2009, 94, .	3.3	106
12	Activation of New Raman Modes by Inversion Symmetry Breaking in Type II Weyl Semimetal Candidate Tâ€²-MoTe₂. Nano Letters, 2016, 16, 5852-5860.	9.1	102
13	Carrier-induced antiferromagnet of graphene islands embedded in hexagonal boron nitride. Physical Review B, 2011, 84, .	3.2	73
14	Manganese Doping of MoSe₂ Promotes Active Defect Sites for Hydrogen Evolution. ACS Applied Materials & Interfaces, 2019, 11, 25155-25162.	8.0	70
15	CO Adsorption on Defective Graphene-Supported Pt₁₃ Nanoclusters. Journal of Physical Chemistry C, 2013, 117, 19927-19933.	3.1	62
16	Comparing time-dependent density functional theory with many-body perturbation theory for semiconductors: Screened range-separated hybrids and the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m plus Bethe-Salpeter approach. Physical Review Materials, 2019, 3, .	2.4	61
17	Mechanical properties of irradiated single-layer graphene. Applied Physics Letters, 2013, 103, 013102.	3.3	59
18	Adsorption of CO on Low-Energy, Low-Symmetry Pt Nanoparticles: Energy Decomposition Analysis and Prediction via Machine-Learning Models. Journal of Physical Chemistry C, 2017, 121, 5612-5619.	3.1	58

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19	Protective molecular passivation of black phosphorus. Npj 2D Materials and Applications, 2017, 1, .	7.9	52
20	Effect of atomic scale plasticity on hydrogen diffusion in iron: Quantum mechanically informed and on-the-fly kinetic Monte Carlo simulations. Journal of Materials Research, 2008, 23, 2757-2773.	2.6	50
21	Electronic structure of oxygen-terminated zigzag graphene nanoribbons: A hybrid density functional theory study. Physical Review B, 2010, 81, .	3.2	50
22	The Intrinsic Mechanical Properties of Rubrene Single Crystals. Advanced Materials, 2012, 24, 5548-5552.	21.0	50
23	Three-dimensional simulations of self-assembly of hut-shaped Siâ€“Ge quantum dots. Journal of Applied Physics, 2004, 95, 7813-7824.	2.5	46
24	Influence of Support Effects on CO Oxidation Kinetics on CO-Saturated Graphene-Supported Pt₁₃ Nanoclusters. Journal of Physical Chemistry C, 2015, 119, 8703-8710.	3.1	46
25	A Comparison of the Elastic Properties of Graphene- and Fullerene-Reinforced Polymer Composites: The Role of Filler Morphology and Size. Scientific Reports, 2016, 6, 31735.	3.3	46
26	Au-MoS₂ Hybrids as Hydrogen Evolution Electrocatalysts. ACS Applied Energy Materials, 2019, 2, 6043-6050.	5.1	43
27	Elastic properties of graphene nanomeshes. Applied Physics Letters, 2014, 104, .	3.3	42
28	Raman scattering and anomalous Stokesâ€“anti-Stokes ratio in MoTe2 atomic layers. Scientific Reports, 2016, 6, 28024.	3.3	41
29	First-Principles Predictions of Structureâ€“Function Relationships of Graphene-Supported Platinum Nanoclusters. Journal of Physical Chemistry C, 2016, 120, 11899-11909.	3.1	40
30	Promoting Active Sites for Hydrogen Evolution in MoSe₂ via Transition-Metal Doping. Journal of Physical Chemistry C, 2020, 124, 12324-12336.	3.1	38
31	Density-Functional Tight-Binding Simulations of Curvature-Controlled Layer Decoupling and Band-Gap Tuning in Bilayer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>MoS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Physical Review Letters, 2014, 112, 186802.	7.8	36
32	On the evolution of faceted grain-boundary grooves by surface diffusion. Acta Materialia, 2005, 53, 2943-2956.	7.9	35
33	Orbital-free density functional theory simulations of dislocations in aluminum. Philosophical Magazine, 2009, 89, 3195-3213.	1.6	34
34	Tetrathiafulvalene-containing polymers for simultaneous non-covalent modification and electronic modulation of MoS₂ nanomaterials. Chemical Science, 2016, 7, 4698-4705.	7.4	34
35	Aqueous-phase hydrodeoxygenation of highly oxygenated aromatics on platinum. Green Chemistry, 2014, 16, 675-682.	9.0	31
36	A variational approach to nonlinear dynamics of nanoscale surface modulations. Surface Science, 2003, 529, 365-383.	1.9	29

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37	Mechanical behavior and fracture of graphene nanomeshes. Journal of Applied Physics, 2015, 117, .	2.5	28
38	Coupled Quantumâ€“Atomistic and Quantumâ€“Continuum Mechanics Methods in Materials Research. MRS Bulletin, 2007, 32, 913-918.	3.5	25
39	Enhancing Lightâ€“Matter Interactions in MoS₂ by Copper Intercalation. Advanced Materials, 2021, 33, e2008779.	21.0	25
40	A discrete mechanics approach to dislocation dynamics in BCC crystals. Journal of the Mechanics and Physics of Solids, 2007, 55, 615-647.	4.8	23
41	Nanotubes from Oxide-Based Misfit Family: The Case of Calcium Cobalt Oxide. ACS Nano, 2016, 10, 6248-6256.	14.6	23
42	Density Functional Theory Studies of the Methanol Decomposition Reaction on Graphene-Supported Pt₁₃ Nanoclusters. Journal of Physical Chemistry C, 2016, 120, 17408-17417.	3.1	23
43	Self-Consistent Charge Density-Functional Tight-Binding Parametrization for Ptâ€“Ru Alloys. Journal of Physical Chemistry A, 2017, 121, 2497-2502.	2.5	23
44	Substrate-induced magnetism in epitaxial graphene buffer layers. Nanotechnology, 2009, 20, 275705.	2.6	22
45	Analysis of vacancy-induced amorphization of single-layer graphene. Applied Physics Letters, 2012, 100, 203105.	3.3	22
46	Edge-stress-induced spontaneous twisting of graphene nanoribbons. Journal of Applied Physics, 2012, 111, 054302.	2.5	21
47	Edge stresses of non-stoichiometric edges in two-dimensional crystals. Applied Physics Letters, 2012, 100, .	3.3	21
48	Relaxation kinetics of nano-ripples on Cu(001) surface. Physical Review B, 2004, 70, .	3.2	20
49	Transferable screened range-separated hybrids for layered materials: The cases of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> h-BN. Physical Review Materials, 2019, 3, .	2.4	20
50	Influence of Step-Edge Barriers on the Morphological Relaxation of Nanoscale Ripples on Crystal Surfaces. Physical Review Letters, 2004, 92, 256101.	7.8	19
51	Multiscale Shear-Lag Analysis of Stiffness Enhancement in Polymerâ€“Graphene Nanocomposites. ACS Applied Materials & Interfaces, 2017, 9, 23092-23098.	8.0	19
52	The role of water in the adsorption of oxygenated aromatics on Pt and Pd. Journal of Computational Chemistry, 2013, 34, 60-66.	3.3	18
53	Electronic Tuning of Monolayer Graphene with Polymeric â€œZwitteristsâ€. ACS Nano, 2021, 15, 2762-2770.	14.6	17
54	Tuned and screened range-separated hybrid density functional theory for describing electronic and optical properties of defective gallium nitride. Physical Review Materials, 2020, 4, .	2.4	17

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55	The elastic constants of rubrene determined by Brillouin scattering and density functional theory. Applied Physics Letters, 2017, 110, .	3.3	15
56	Identifying a New Pathway for Nitrogen Reduction Reaction on Fe-Doped MoS₂ by the Coadsorption of Hydrogen and N₂. Journal of Physical Chemistry C, 2021, 125, 19980-19990.	3.1	14
57	Combining 2D inorganic semiconductors and organic polymers at the frontier of the hardâ€“soft materials interface. Journal of Materials Chemistry C, 2017, 5, 11158-11164.	5.5	13
58	Structure and Morphology of Light-Reflecting Synthetic and Biogenic Polymorphs of Isoxanthopterin: A Comparison. Chemistry of Materials, 2019, 31, 4479-4489.	6.7	12
59	Interactions between Transition-Metal Surfaces and MoS₂ Monolayers: Implications for Hydrogen Evolution and CO₂ Reduction Reactions. Journal of Physical Chemistry C, 2020, 124, 20116-20124.	3.1	12
60	Mechanical properties of hydrogenated electron-irradiated graphene. Journal of Applied Physics, 2016, 120, 124301.	2.5	11
61	Tuning coreâ€“shell interactions in tungsten carbideâ€“Pt nanoparticles for the hydrogen evolution reaction. Physical Chemistry Chemical Physics, 2018, 20, 23262-23271.	2.8	11
62	Lithographically Patterned Functional Polymerâ€“Graphene Hybrids for Nanoscale Electronics. ACS Nano, 2018, 12, 1928-1933.	14.6	10
63	Fracture in nanolamellar materials: Continuum and atomistic models with application to titanium aluminides. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 2002, 82, 2397-2417.	0.6	9
64	Growth and Ordering of Si-Ge Quantum Dots on Strain Patterned Substrates. Journal of Engineering Materials and Technology, Transactions of the ASME, 2005, 127, 434-443.	1.4	9
65	Strontium Cobalt Oxide Misfit Nanotubes. Chemistry of Materials, 2016, 28, 9150-9157.	6.7	9
66	Thermal conductivity of electron-irradiated graphene. Applied Physics Letters, 2017, 111, .	3.3	9
67	Electronic structure of electron-irradiated graphene and effects of hydrogen passivation. Materials Research Express, 2018, 5, 115603.	1.6	9
68	Effects of pore morphology and pore edge termination on the mechanical behavior of graphene nanomeshes. Journal of Applied Physics, 2019, 126, 164306.	2.5	9
69	Molecular-Dynamics Simulations on Nanoindentation of Graphene-Diamond Composite Superstructures in Interlayer-Bonded Twisted Bilayer Graphene: Implications for Mechanical Metamaterials. ACS Applied Nano Materials, 2021, 4, 8611-8625.	5.0	9
70	Optoelectronic properties of calcium cobalt oxide misfit nanotubes. Applied Physics Letters, 2018, 113, .	3.3	7
71	Structure-properties relations in graphene derivatives and metamaterials obtained by atomic-scale modeling. Molecular Simulation, 2019, 45, 1173-1202.	2.0	6
72	Bidirectional Electronic Tuning of Single-Layer MoS₂ with Conjugated Organochalcogens. Journal of Physical Chemistry C, 2019, 123, 1506-1511.	3.1	6

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73	Molecular-Dynamics Analysis of Nanoindentation of Graphene Nanomeshes: Implications for 2D Mechanical Metamaterials. ACS Applied Nano Materials, 2020, 3, 3613-3624.	5.0	6
74	A spectral method for the nonconserved surface evolution of nanocrystalline gratings below the roughening transition. Journal of Applied Physics, 2005, 97, 114312.	2.5	3
75	Dynamics of nanoscale ripple relaxation on alloy surfaces. Physical Review E, 2008, 77, 021601.	2.1	3
76	Polarization-Driven Asymmetric Electronic Response of Monolayer Graphene to Polymer Zwitterions Probed from Both Sides. ACS Applied Materials & Interfaces, 2021, 13, 47945-47953.	8.0	3
77	Kinetic composition locking on faceted alloy surfaces. Acta Materialia, 2009, 57, 196-201.	7.9	2
78	Firstâ€principles Studies of the Electronic and Thermoelectric Properties of Misfit Layered Phases of Calcium Cobaltite. Israel Journal of Chemistry, 2017, 57, 522-528.	2.3	2
79	Fast Automated Phase Differentiation in Industrial Stainless Steel by Combining Low-Loss EELS Experiments with Machine Learning-based Algorithms. Microscopy and Microanalysis, 2021, 27, 34-36.	0.4	2
80	Fracture in nanolamellar materials: continuum and atomistic models with application to titanium aluminides. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 2002, 82, 2397-2417.	0.6	2
81	Non-asymptotic quantum scattering theory to design high-mobility lateral transition-metal dichalcogenide heterostructures. Journal of Applied Physics, 2022, 131, .	2.5	2
82	Light Emission from Atomic Monolayers in a One-Dimensional Microcavity. , 2014, , .		0
83	Discrete Dislocation Dynamics in Crystals. Mathematics in Industry, 2008, , 387-391.	0.3	0