Ashwin Ramasubramaniam

List of Publications by Year in Descending Order

82 papers	6,686 citations	30 h-index	81 g-index
86 ext. papers	7,541 ext. citations	5.9 avg, IF	6.66 L-index

#	Paper	IF	Citations
82	Non-asymptotic quantum scattering theory to design high-mobility lateral transition-metal dichalcogenide heterostructures. *Journal of Applied Physics*, **2022**, 131, 174302	2.5	0
81	Polarization-Driven Asymmetric Electronic Response of Monolayer Graphene to Polymer Zwitterions Probed from Both Sides. *ACS Applied Materials & Interfaces*, **2021**, 13, 47945-47953	9.5	1
80	Enhancing Light-Matter Interactions in MoS by Copper Intercalation. *Advanced Materials*, **2021**, 33, e2008779	27	10
79	Electronic Tuning of Monolayer Graphene with Polymeric "Zwitterists". *ACS Nano*, **2021**, 15, 2762-2770	16.7	11
78	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	0.5	1
77	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	5.6	2
76	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	3.8	6
75	Promoting Active Sites for Hydrogen Evolution in MoSe2 via Transition-Metal Doping. *Journal of Physical Chemistry C*, **2020**, 124, 12324-12336	3.8	21
74	Molecular-Dynamics Analysis of Nanoindentation of Graphene Nanomeshes: Implications for 2D Mechanical Metamaterials. *ACS Applied Nano Materials*, **2020**, 3, 3613-3624	5.6	3
73	Tuned and screened range-separated hybrid density functional theory for describing electronic and optical properties of defective gallium nitride. *Physical Review Materials*, **2020**, 4,	3.2	7
72	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	3.8	4
71	Manganese Doping of MoSe Promotes Active Defect Sites for Hydrogen Evolution. *ACS Applied Materials & Interfaces*, **2019**, 11, 25155-25162	9.5	38
70	Structure-properties relations in graphene derivatives and metamaterials obtained by atomic-scale modeling. *Molecular Simulation*, **2019**, 45, 1173-1202	2	5
69	Structure and Morphology of Light-Reflecting Synthetic and Biogenic Polymorphs of Isoxanthopterin: A Comparison. *Chemistry of Materials*, **2019**, 31, 4479-4489	9.6	7
68	Au-MoS2 Hybrids as Hydrogen Evolution Electrocatalysts. *ACS Applied Energy Materials*, **2019**, 2, 6043-6050	5.4	23
67	Comparing time-dependent density functional theory with many-body perturbation theory for semiconductors: Screened range-separated hybrids and the GW plus Bethe-Salpeter approach. *Physical Review Materials*, **2019**, 3,	3.2	36
66	Transferable screened range-separated hybrids for layered materials: The cases of MoS2 and h-BN. *Physical Review Materials*, **2019**, 3,	3.2	10

65	Effects of pore morphology and pore edge termination on the mechanical behavior of graphene nanomeshes. *Journal of Applied Physics*, **2019**, 126, 164306	2.5	7
64	Bidirectional Electronic Tuning of Single-Layer MoS2 with Conjugated Organochalcogens. *Journal of Physical Chemistry C*, **2019**, 123, 1506-1511	3.8	4
63	Lithographically Patterned Functional Polymer-Graphene Hybrids for Nanoscale Electronics. *ACS Nano*, **2018**, 12, 1928-1933	16.7	7
62	Optoelectronic properties of calcium cobalt oxide misfit nanotubes. *Applied Physics Letters*, **2018**, 113, 031102	3.4	4
61	Electronic structure of electron-irradiated graphene and effects of hydrogen passivation. *Materials Research Express*, **2018**, 5, 115603	1.7	4
60	Tuning core-shell interactions in tungsten carbide-Pt nanoparticles for the hydrogen evolution reaction. *Physical Chemistry Chemical Physics*, **2018**, 20, 23262-23271	3.6	8
59	The elastic constants of rubrene determined by Brillouin scattering and density functional theory. *Applied Physics Letters*, **2017**, 110, 071903	3.4	11
58	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	3.8	38
57	Multiscale Shear-Lag Analysis of Stiffness Enhancement in Polymer-Graphene Nanocomposites. *ACS Applied Materials & Interfaces*, **2017**, 9, 23092-23098	9.5	12
56	Protective molecular passivation of black phosphorus. *Npj 2D Materials and Applications*, **2017**, 1,	8.8	46
55	Self-Consistent Charge Density-Functional Tight-Binding Parametrization for Pt-Ru Alloys. *Journal of Physical Chemistry A*, **2017**, 121, 2497-2502	2.8	16
54	Thermal conductivity of electron-irradiated graphene. *Applied Physics Letters*, **2017**, 111, 163101	3.4	7
53	Combining 2D inorganic semiconductors and organic polymers at the frontier of the hard/soft materials interface. *Journal of Materials Chemistry C*, **2017**, 5, 11158-11164	7.1	10
52	First-principles Studies of the Electronic and Thermoelectric Properties of Misfit Layered Phases of Calcium Cobaltite. *Israel Journal of Chemistry*, **2017**, 57, 522-528	3.4	1
51	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	4.9	36
50	Raman scattering and anomalous Stokes-anti-Stokes ratio in MoTe2 atomic layers. *Scientific Reports* , **2016**, 6, 28024	4.9	35
49	Activation of New Raman Modes by Inversion Symmetry Breaking in Type II Weyl Semimetal Candidate T'-MoTe2. *Nano Letters*, **2016**, 16, 5852-60	11.5	77
48	Density Functional Theory Studies of the Methanol Decomposition Reaction on Graphene-Supported Pt13 Nanoclusters. *Journal of Physical Chemistry C*, **2016**, 120, 17408-17417	3.8	19

47	First-Principles Predictions of Structure–Function Relationships of Graphene-Supported Platinum Nanoclusters. *Journal of Physical Chemistry C*, **2016**, 120, 11899-11909	3.8	32
46	Mechanical properties of hydrogenated electron-irradiated graphene. *Journal of Applied Physics*, **2016**, 120, 124301	2.5	11
45	Strontium Cobalt Oxide Misfit Nanotubes. *Chemistry of Materials*, **2016**, 28, 9150-9157	9.6	6
44	Nanotubes from Oxide-Based Misfit Family: The Case of Calcium Cobalt Oxide. *ACS Nano*, **2016**, 10, 6248-56	13.7	19
43	Tetrathiafulvalene-containing polymers for simultaneous non-covalent modification and electronic modulation of MoS nanomaterials. *Chemical Science*, **2016**, 7, 4698-4705	9.4	29
42	Influence of Support Effects on CO Oxidation Kinetics on CO-Saturated Graphene-Supported Pt13 Nanoclusters. *Journal of Physical Chemistry C*, **2015**, 119, 8703-8710	3.8	40
41	Mechanical behavior and fracture of graphene nanomeshes. *Journal of Applied Physics*, **2015**, 117, 024302	2.5	23
40	Elastic properties of graphene nanomeshes. *Applied Physics Letters*, **2014**, 104, 141911	3.4	33
39	Aqueous-phase hydrodeoxygenation of highly oxygenated aromatics on platinum. *Green Chemistry*, **2014**, 16, 675-682	10	27
38	Density-functional tight-binding simulations of curvature-controlled layer decoupling and band-gap tuning in bilayer MoS2. *Physical Review Letters*, **2014**, 112, 186802	7.4	32
37	Ab initio studies of thermodynamic and electronic properties of phosphorene nanoribbons. *Physical Review B*, **2014**, 90,	3.3	112
36	Two-dimensional material nanophotonics. *Nature Photonics*, **2014**, 8, 899-907	33.9	1805
35	CO Adsorption on Defective Graphene-Supported Pt13 Nanoclusters. *Journal of Physical Chemistry C*, **2013**, 117, 19927-19933	3.8	54
34	Mn-doped monolayer MoS2: An atomically thin dilute magnetic semiconductor. *Physical Review B*, **2013**, 87,	3.3	351
33	The role of water in the adsorption of oxygenated aromatics on Pt and Pd. *Journal of Computational Chemistry*, **2013**, 34, 60-6	3.5	17
32	Mechanical properties of irradiated single-layer graphene. *Applied Physics Letters*, **2013**, 103, 013102	3.4	52
31	Binding of Pt Nanoclusters to Point Defects in Graphene: Adsorption, Morphology, and Electronic Structure. *Journal of Physical Chemistry C*, **2012**, 116, 6543-6555	3.8	193
30	Large excitonic effects in monolayers of molybdenum and tungsten dichalcogenides. *Physical Review B*, **2012**, 86,	3.3	1061

29	Edge stresses of non-stoichiometric edges in two-dimensional crystals. *Applied Physics Letters*, **2012**, 100, 251906	3.4	17
28	The intrinsic mechanical properties of rubrene single crystals. *Advanced Materials*, **2012**, 24, 5548-52	24	45
27	Analysis of vacancy-induced amorphization of single-layer graphene. *Applied Physics Letters*, **2012**, 100, 203105	3.4	19
26	Edge-stress-induced spontaneous twisting of graphene nanoribbons. *Journal of Applied Physics*, **2012**, 111, 054302	2.5	20
25	Tunable band gaps in bilayer graphene-BN heterostructures. *Nano Letters*, **2011**, 11, 1070-5	11.5	199
24	Tunable band gaps in bilayer transition-metal dichalcogenides. *Physical Review B*, **2011**, 84,	3.3	442
23	Carrier-induced antiferromagnet of graphene islands embedded in hexagonal boron nitride. *Physical Review B*, **2011**, 84,	3.3	69
22	Hydrogen bond networks in graphene oxide composite paper: structure and mechanical properties. *ACS Nano*, **2010**, 4, 2300-6	16.7	568
21	Electronic structure of oxygen-terminated zigzag graphene nanoribbons: A hybrid density functional theory study. *Physical Review B*, **2010**, 81,	3.3	44
20	Kinetic composition locking on faceted alloy surfaces. *Acta Materialia*, **2009**, 57, 196-201	8.4	2
19	Substrate-induced magnetism in epitaxial graphene buffer layers. *Nanotechnology*, **2009**, 20, 275705	3.4	19
18	Interatomic potentials for hydrogen in Iron based on density functional theory. *Physical Review B*, **2009**, 79,	3.3	126
17	Edge elastic properties of defect-free single-layer graphene sheets. *Applied Physics Letters*, **2009**, 94, 101904	3.4	102
16	Orbital-free density functional theory simulations of dislocations in aluminum. *Philosophical Magazine*, **2009**, 89, 3195-3213	1.6	32
15	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	2.5	46
14	Dynamics of nanoscale ripple relaxation on alloy surfaces. *Physical Review E*, **2008**, 77, 021601	2.4	3
13	Edge-stress-induced warping of graphene sheets and nanoribbons. *Physical Review Letters*, **2008**, 101, 245501	7.4	298
12	Discrete Dislocation Dynamics in Crystals. *Mathematics in Industry*, **2008**, 387-391	0.2	

11	A discrete mechanics approach to dislocation dynamics in BCC crystals. *Journal of the Mechanics and Physics of Solids*, **2007**, 55, 615-647	5	22
10	Coupled Quantum-Atomistic and Quantum-Continuum Mechanics Methods in Materials Research. *MRS Bulletin*, **2007**, 32, 913-918	3.2	21
9	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	1.8	7
8	On the evolution of faceted grain-boundary grooves by surface diffusion. *Acta Materialia*, **2005**, 53, 2943-2956	3.4	30
7	A spectral method for the nonconserved surface evolution of nanocrystalline gratings below the roughening transition. *Journal of Applied Physics*, **2005**, 97, 114312	2.5	2
6	Relaxation kinetics of nano-ripples on Cu(001) surface. *Physical Review B*, **2004**, 70,	3.3	17
5	Influence of step-edge barriers on the morphological relaxation of nanoscale ripples on crystal surfaces. *Physical Review Letters*, **2004**, 92, 256101	7.4	17
4	Three-dimensional simulations of self-assembly of hut-shaped Si-Ge quantum dots. *Journal of Applied Physics*, **2004**, 95, 7813-7824	2.5	46
3	A variational approach to nonlinear dynamics of nanoscale surface modulations. *Surface Science*, **2003**, 529, 365-383	1.8	24
2	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		9
1	Fracture in nanolamellar materials: Continuum and atomistic models with application to titanium aluminides		1