Manish Jain

List of Publications by Year
in descending order

90 papers	4,367 citations	147801 31 h-index	110387 64 g-index
92 all docs	92 docs citations	92 times ranked	5173 citing authors

#	Article	IF	Citations
1	Twister: Construction and structural relaxation of commensurate moirÃ© superlattices. Computer Physics Communications, 2022, 271, 108184.	7.5	16
2	MoirÃ© induced topology and flat bands in twisted bilayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">WSe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> : A first-principles study. Physical Review B, 2022, 105, .	3.2	11
3	Breakdown of semiclassical description of thermoelectricity in near-magic angle twisted bilayer graphene. Nature Communications, 2022, 13, 1522.	12.8	12
4	Tunable lattice thermal conductivity of twisted bilayer MoS₂. Physical Chemistry Chemical Physics, 2022, 24, 13860-13868.	2.8	3
5	Molybdenum and Tungsten Di-sulfides: First Principles Investigation of Adatom Attachment and Diffusion on c-plane Alpha Sapphire and Correlation with Growth. Crystal Growth and Design, 2022, 22, 4708-4720.	3.0	4
6	Oxygen vacancy induced electronic structure modification of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>KTaO</mml:mi><mml:mn>3</mml:mn></mml:msub></m Physical Review B, 2021, 103, .	3.2	23
7	Population analysis with Wannier orbitals. Journal of Chemical Physics, 2021, 154, 104111.	3.0	3
8	Fine-tuning the DNA conductance by intercalation of drug molecules. Physical Review E, 2021, 103, 032411.	2.1	5
9	Reconstruction of moirÃ© lattices in twisted transition metal dichalcogenide bilayers. Physical Review B, 2021, 103, .	3.2	22
10	Spontaneous Time-Reversal Symmetry Breaking at Individual Grain Boundaries in Graphene. Physical Review Letters, 2021, 126, 206803.	7.8	7
11	Anomalous electrical transport in orientationally controlled trinary hybrids of graphene and twisted bilayer molybdenum disulphide. Bulletin of Materials Science, 2021, 44, 1.	1.7	0
12	Anisotropic Charge Transport in Nanoscale DNA Wire. Journal of Physical Chemistry C, 2020, 124, 16763-16772.	3.1	8
13	Origin and evolution of ultraflat bands in twisted bilayer transition metal dichalcogenides: Realization of triangular quantum dots. Physical Review B, 2020, 102, .	3.2	62
14	First-principles theoretical analysis and electron energy loss spectroscopy of vacancy defects in bulk and nonpolar (101Â¯) surface of GaN. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2020, 38, .	2.1	4
15	Multiscale modelling reveals higher charge transport efficiencies of DNA relative to RNA independent of mechanism. Nanoscale, 2020, 12, 18750-18760.	5.6	10
16	Misorientation-Controlled Cross-Plane Thermoelectricity in Twisted Bilayer Graphene. Physical Review Letters, 2020, 125, 226802.	7.8	26
17	Anharmonicity in Raman-active phonon modes in atomically thin <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></ Physical Review B, 2020, 101, .	3.2	18
18	Oxygen Vacancyâ€Induced Topological Hall Effect in a Nonmagnetic Band Insulator. Advanced Quantum Technologies, 2020, 3, 2000021.	3.9	9

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19	Evolution of high-frequency Raman modes and their doping dependence in twisted bilayer MoS₂. Nanoscale, 2020, 12, 17272-17280.	5.6	23
20	Native point defects in mono and bilayer phosphorene. Physical Review Materials, 2020, 4, .	2.4	9
21	Phonons in twisted transition-metal dichalcogenide bilayers: Ultrasoft phasons and a transition from a superlubric to a pinned phase. Physical Review Research, 2020, 2, .	3.6	45
22	Large intrinsic magnetization in an epitaxial BiFeO3/NdGaO3system. Europhysics Letters, 2019, 126, 57003.	2.0	1
23	Thermodynamically stable octahedral MoS ₂ in van der Waals hetero-bilayers. 2D Materials, 2019, 6, 041002.	4.4	9
24	Polarization discontinuity driven two dimensional electron gas at A2Mo3O8/B2Mo3O8 (A, B: Zn, Mg,) Tj ETQq0 0 0 rgBT /Overlock 10 T	2.5	2
25	Kolmogorovâ€“Crespi Potential For Multilayer Transition-Metal Dichalcogenides: Capturing Structural Transformations in MoirÃ© Superlattices. Journal of Physical Chemistry C, 2019, 123, 9770-9778.	3.1	60
26	Electrical and optical properties of low-bandgap oxide Zn2Mo3O8 for optoelectronic applications. Thin Solid Films, 2019, 677, 95-102.	1.8	5
27	Reversible defect engineering in graphene grain boundaries. Nature Communications, 2019, 10, 1090.	12.8	44
28	Electronic structure and optical properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>F</mml:mi></mml:math> centers in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi></mml:math> -alumina. Physical Review B, 2019, 99, .	3.2	10
29	Spin density encodes intramolecular singlet exciton fission in pentacene dimers. Nature Communications, 2019, 10, 33.	12.8	34
30	Temperature-dependent layer breathing modes in two-dimensional materials. Physical Review B, 2018, 97, .	3.2	8
31	Electronic and Thermoelectric Properties of Transition Metal Substituted Tetrahedrites. Journal of Physical Chemistry C, 2018, 122, 8735-8749.	3.1	45
32	CoFFEE: Corrections For Formation Energy and Eigenvalues for charged defect simulations. Computer Physics Communications, 2018, 226, 114-126.	7.5	50
33	Electronic and thermoelectric properties of Zn and Se double substituted tetrahedrite. Physical Chemistry Chemical Physics, 2018, 20, 28667-28677.	2.8	16
34	Efficient hybrid and screened hybrid density functional calculations of carbon and silicon nanostructures electronic properties. , 2018, , .		0
35	Ultraflatbands and Shear Solitons in MoirÃ© Patterns of Twisted Bilayer Transition Metal Dichalcogenides. Physical Review Letters, 2018, 121, 266401.	7.8	297
36	PASTA: Python Algorithms for Searching Transition stAtes. Computer Physics Communications, 2018, 233, 261-268.	7.5	15

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37	Opening of large band gaps in metallic carbon nanotubes by mannose-functionalized dendrimers: experiments and theory. Journal of Materials Chemistry C, 2018, 6, 6483-6488.	5.5	10
38	Substrate screening effects on the quasiparticle band gap and defect charge transition levels in <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></mm Physical Review Materials, 2018, 2, .	2.4	64
39	Quantized edge modes in atomic-scale point contacts in graphene. Nature Nanotechnology, 2017, 12, 564-568.	31.5	18
40	Optical Properties of Zn2Mo3O8: Combination of Theoretical and Experimental Study. Journal of Physical Chemistry C, 2017, 121, 24766-24773.	3.1	15
41	Size dependent electronic properties of silicon quantum dotsâ€"An analysis with hybrid, screened hybrid and local density functional theory. Computer Physics Communications, 2017, 221, 95-101.	7.5	9
42	Origin of the thermal expansion anomaly in layered <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Bi</mml:mi><mml:mn>2</mml:mn></mml:n mathvariant="normal">X</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> topological insulators: Ultrafast time-resolved pump-probe experiments and theory. Physical Review B, 2017, 96, .	3.2	5
43	Density-Functional Theory of the Fractional Quantum Hall Effect. Physical Review Letters, 2017, 118, 196802.	7.8	7
44	Origin of layer dependence in band structures of two-dimensional materials. Physical Review B, 2017, 95, .	3.2	26
45	Asymptotic behavior and interpretation of virtual states: The effects of confinement and of basis sets. Journal of Chemical Physics, 2016, 144, 084104.	3.0	6
46	Quasiparticle band structure and optical properties of hexagonal-YMnO3. Journal of Applied Physics, 2016, 120, .	2.5	10
47	First-principles investigation of cubicBaRuO3: A Hund's metal. Physical Review B, 2016, 94, .	3.2	9
48	Charge Transport in Dendrimer Melts Using Multiscale Modeling Simulation. Journal of Physical Chemistry B, 2016, 120, 9142-9151.	2.6	11
49	Efficient Computation of the Hartreeâ€"Fock Exchange in Real-Space with Projection Operators. Journal of Chemical Theory and Computation, 2016, 12, 3614-3622.	5.3	21
50	Magnitude and Origin of Electrical Noise at Individual Grain Boundaries in Graphene. Nano Letters, 2016, 16, 562-567.	9.1	39
51	Structural-modulation-driven spin canting and reentrant glassy magnetic phase in ferromagneticLu2MnNiO6. Physical Review B, 2015, 91, .	3.2	32
52	Solid-state optical absorption from optimally tuned time-dependent range-separated hybrid density functional theory. Physical Review B, 2015, 92, .	3.2	210
53	Ultra-sensitive pressure dependence of bandgap of rutile-GeO2 revealed by many body perturbation theory. Journal of Chemical Physics, 2015, 143, 064703.	3.0	9
54	Probing 2D black phosphorus by quantum capacitance measurements. Nanotechnology, 2015, 26, 485704.	2.6	11

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55	Thermoelectric properties of Co substituted synthetic tetrahedrite. Acta Materialia, 2015, 100, 266-274.	7.9	96
56	Microscopic origin of low frequency noise in MoS2 field-effect transistors. APL Materials, 2014, 2, .	5.1	57
57	Synergistic Effect of Mo + Cu Codoping on the Photocatalytic Behavior of Metastable TiO₂ Solid Solutions. Journal of Physical Chemistry C, 2014, 118, 29788-29795.	3.1	20
58	Improved quasiparticle wave functions and mean field for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mml:msub></mml:mrow></mml:math> Initialization with the COHSEX operator. Physical Review B, 2014, 90, .	3.2	14
59	First-principles<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>DFT</mml:mi><mml:mo>+</mml:mo><mml:mi>G</mml:mi></mml:mrow></mml:math> of oxygen vacancies in rutile<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>TiO</mml:mtext><mml:mn>2</mml:mn></mml:msub></mml:math> Physical Review B, 2014, 89, .	3.2	80
60	Gap renormalization of molecular crystals from density-functional theory. Physical Review B, 2013, 88, .	3.2	239
61	Coulomb-hole summations and energies for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>calculations with limited number of empty orbitals: A modified static remainder approach. Physical Review B, 2013, 87, .	3.2	149
62	Mechanism for optical initialization of spin in NV<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mrow /><mml:mo>â^’</mml:mo></mml:msup></mml:math>center in diamond. Physical Review B, 2012, 86, .	3.2	53
63	First-Principles Calculations of Quasiparticle Excitations of Open-Shell Condensed Matter Systems. Physical Review Letters, 2012, 109, 036406.	7.8	29
64	BerkeleyGW: A massively parallel computer package for the calculation of the quasiparticle and optical properties of materials and nanostructures. Computer Physics Communications, 2012, 183, 1269-1289.	7.5	706
65	Quasiparticle Excitations and Charge Transition Levels of Oxygen Vacancies in Hafnia. Physical Review Letters, 2011, 107, 216803.	7.8	54
66	Simple Approximate Physical Orbitals for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:math>Quasiparticle Calculations. Physical Review Letters, 2011, 107, 186404.	7.8	63
67	Reliability of Hybrid Functionals in Predicting Band Gaps. Physical Review Letters, 2011, 107, 216806.	7.8	150
68	Time-dependent density functional theory calculations for the Stokes shift in hydrogenated silicon clusters. Physical Review B, 2010, 81, .	3.2	16
69	Viscoelastic effect on acoustic band gaps in polymer-fluid composites. Modelling and Simulation in Materials Science and Engineering, 2009, 17, 075013.	2.0	24
70	Application of time-dependent density-functional theory to molecules and nanostructures. Computational and Theoretical Chemistry, 2009, 914, 115-129.	1.5	13
71	Structure of Iron-Containing Nitrogenated Carbon. Journal of Physical Chemistry C, 2008, 112, 9777-9782.	3.1	5
72	Elastic and viscoelastic effects in rubber/air acoustic band gap structures: A theoretical and experimental study. Journal of Applied Physics, 2008, 104, .	2.5	61

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73	Efficient first-principles calculations of the electronic structure of periodic systems. Computer Physics Communications, 2007, 177, 339-347.	7.5	18
74	In Search for Structure of Active Site in Iron-Based Oxygen Reduction Electrocatalysts. Journal of Physical Chemistry B, 2006, 110, 4179-4185.	2.6	28
75	PARSEC â€“ the pseudopotential algorithm for real-space electronic structure calculations: recent advances and novel applications to nano-structures. Physica Status Solidi (B): Basic Research, 2006, 243, 1063-1079.	1.5	285
76	Electronic structure and spin polarization of MnGaP. Applied Physics Letters, 2004, 85, 2014-2016.	3.3	5
77	Real-space pseudopotential method for computing the electronic properties of periodic systems. Physical Review B, 2004, 69, .	3.2	83
78	Formation of intermetallic compounds in the Niâ€“Alâ€“Si ternary system. Materials Characterization, 2003, 51, 243-257.	4.4	38
79	Parallel implementation of time-dependent density functional theory. Computer Physics Communications, 2003, 156, 22-42.	7.5	36
80	Using real space pseudopotentials for the electronic structure problem. Handbook of Numerical Analysis, 2003, 10, 613-637.	1.8	9
81	Simulating Semiconductor Liquids with Ab Initio Pseudopotentials and Quantum Forces. Springer Proceedings in Physics, 2003, , 149-162.	0.2	1
82	Hybridization and Bond-Orbital Components in Site-Specific X-Ray Photoelectron Spectra of RutileTiO2. Physical Review Letters, 2002, 89, 077401.	7.8	126
83	Electronic structure and spin polarization ofMnxGa1â^'xN. Physical Review B, 2002, 66, .	3.2	214
84	First principles simulations of SiGe for the liquid and amorphous states. Journal of Chemical Physics, 2002, 117, 3476-3483.	3.0	23
85	Ab initiosimulations of liquid semiconductors using the pseudopotential-density functional method. Journal of Physics Condensed Matter, 2001, 13, R817-R854.	1.8	29
86	Partial density of occupied valence states by x-ray standing waves and high-resolution photoelectron spectroscopy. Physical Review B, 2001, 63, .	3.2	17
87	Ab initiostructures and polarizabilities of sodium clusters. Journal of Chemical Physics, 2001, 115, 4322-4332.	3.0	56
88	Electronic structure and spin polarization of Mn-containing dilute magnetic III-V semiconductors. Physical Review B, 2001, 64, .	3.2	83
89	First-principles simulations of liquid ZnTe. Physical Review B, 2001, 65, .	3.2	16
90	First-principles calculations of liquid CdTe at temperatures above and below the melting point. Physical Review B, 1999, 60, 8640-8649.	3.2	38