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	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
2	Ultraflatbands and Shear Solitons in MoirÃ© Patterns of Twisted Bilayer Transition Metal Dichalcogenides. Physical Review Letters, 2018, 121, 266401.	7.8	297
3	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
4	Gap renormalization of molecular crystals from density-functional theory. Physical Review B, 2013, 88, .	3.2	239
5	Electronic structure and spin polarization ofMnxGa1â^'xN. Physical Review B, 2002, 66, .	3.2	214
6	Solid-state optical absorption from optimally tuned time-dependent range-separated hybrid density functional theory. Physical Review B, 2015, 92, .	3.2	210
7	Reliability of Hybrid Functionals in Predicting Band Gaps. Physical Review Letters, 2011, 107, 216806.	7.8	150
8	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
9	Hybridization and Bond-Orbital Components in Site-Specific X-Ray Photoelectron Spectra of RutileTiO2. Physical Review Letters, 2002, 89, 077401.	7.8	126
10	Thermoelectric properties of Co substituted synthetic tetrahedrite. Acta Materialia, 2015, 100, 266-274.	7.9	96
11	Electronic structure and spin polarization of Mn-containing dilute magnetic III-V semiconductors. Physical Review B, 2001, 64, .	3.2	83
12	Real-space pseudopotential method for computing the electronic properties of periodic systems. Physical Review B, 2004, 69, .	3.2	83
13	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> 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>	3.2	80
14	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></mml:mn> Physical Review Materials, 2018, 2, .	2.4	64
15	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
16	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
17	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
18	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

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19	Microscopic origin of low frequency noise in MoS2 field-effect transistors. APL Materials, 2014, 2, .	5.1	57
20	Ab initiostructures and polarizabilities of sodium clusters. Journal of Chemical Physics, 2001, 115, 4322-4332.	3.0	56
21	Quasiparticle Excitations and Charge Transition Levels of Oxygen Vacancies in Hafnia. Physical Review Letters, 2011, 107, 216803.	7.8	54
22	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
23	CoFFEE: Corrections For Formation Energy and Eigenvalues for charged defect simulations. Computer Physics Communications, 2018, 226, 114-126.	7.5	50
24	Electronic and Thermoelectric Properties of Transition Metal Substituted Tetrahedrites. Journal of Physical Chemistry C, 2018, 122, 8735-8749.	3.1	45
25	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
26	Reversible defect engineering in graphene grain boundaries. Nature Communications, 2019, 10, 1090.	12.8	44
27	Magnitude and Origin of Electrical Noise at Individual Grain Boundaries in Graphene. Nano Letters, 2016, 16, 562-567.	9.1	39
28	First-principles calculations of liquid CdTe at temperatures above and below the melting point. Physical Review B, 1999, 60, 8640-8649.	3.2	38
29	Formation of intermetallic compounds in the Niâ€“Alâ€“Si ternary system. Materials Characterization, 2003, 51, 243-257.	4.4	38
30	Parallel implementation of time-dependent density functional theory. Computer Physics Communications, 2003, 156, 22-42.	7.5	36
31	Spin density encodes intramolecular singlet exciton fission in pentacene dimers. Nature Communications, 2019, 10, 33.	12.8	34
32	Structural-modulation-driven spin canting and reentrant glassy magnetic phase in ferromagneticLu2MnNiO6. Physical Review B, 2015, 91, .	3.2	32
33	Ab initiosimulations of liquid semiconductors using the pseudopotential-density functional method. Journal of Physics Condensed Matter, 2001, 13, R817-R854.	1.8	29
34	First-Principles Calculations of Quasiparticle Excitations of Open-Shell Condensed Matter Systems. Physical Review Letters, 2012, 109, 036406.	7.8	29
35	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
36	Origin of layer dependence in band structures of two-dimensional materials. Physical Review B, 2017, 95, .	3.2	26

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37	Misorientation-Controlled Cross-Plane Thermoelectricity in Twisted Bilayer Graphene. Physical Review Letters, 2020, 125, 226802.	7.8	26
38	Viscoelastic effect on acoustic band gaps in polymer-fluid composites. Modelling and Simulation in Materials Science and Engineering, 2009, 17, 075013.	2.0	24
39	First principles simulations of SiGe for the liquid and amorphous states. Journal of Chemical Physics, 2002, 117, 3476-3483.	3.0	23
40	Evolution of high-frequency Raman modes and their doping dependence in twisted bilayer MoS₂. Nanoscale, 2020, 12, 17272-17280.	5.6	23
41	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></mml:math> Physical Review B, 2021, 103, .	3.2	23
42	Reconstruction of moirÃ© lattices in twisted transition metal dichalcogenide bilayers. Physical Review B, 2021, 103, .	3.2	22
43	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
44	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
45	Efficient first-principles calculations of the electronic structure of periodic systems. Computer Physics Communications, 2007, 177, 339-347.	7.5	18
46	Quantized edge modes in atomic-scale point contacts in graphene. Nature Nanotechnology, 2017, 12, 564-568.	31.5	18
47	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></mml:math> Physical Review B, 2020, 101, .	3.2	18
48	Partial density of occupied valence states by x-ray standing waves and high-resolution photoelectron spectroscopy. Physical Review B, 2001, 63, .	3.2	17
49	First-principles simulations of liquid ZnTe. Physical Review B, 2001, 65, .	3.2	16
50	Time-dependent density functional theory calculations for the Stokes shift in hydrogenated silicon clusters. Physical Review B, 2010, 81, .	3.2	16
51	Electronic and thermoelectric properties of Zn and Se double substituted tetrahedrite. Physical Chemistry Chemical Physics, 2018, 20, 28667-28677.	2.8	16
52	Twister: Construction and structural relaxation of commensurate moirÃ© superlattices. Computer Physics Communications, 2022, 271, 108184.	7.5	16
53	Optical Properties of Zn2Mo3O8: Combination of Theoretical and Experimental Study. Journal of Physical Chemistry C, 2017, 121, 24766-24773.	3.1	15
54	PASTA: Python Algorithms for Searching Transition stAtes. Computer Physics Communications, 2018, 233, 261-268.	7.5	15

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55	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
56	Application of time-dependent density-functional theory to molecules and nanostructures. Computational and Theoretical Chemistry, 2009, 914, 115-129.	1.5	13
57	Breakdown of semiclassical description of thermoelectricity in near-magic angle twisted bilayer graphene. Nature Communications, 2022, 13, 1522.	12.8	12
58	Probing 2D black phosphorus by quantum capacitance measurements. Nanotechnology, 2015, 26, 485704.	2.6	11
59	Charge Transport in Dendrimer Melts Using Multiscale Modeling Simulation. Journal of Physical Chemistry B, 2016, 120, 9142-9151.	2.6	11
60	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
61	Quasiparticle band structure and optical properties of hexagonal-YMnO3. Journal of Applied Physics, 2016, 120, .	2.5	10
62	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
63	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
64	Multiscale modelling reveals higher charge transport efficiencies of DNA relative to RNA independent of mechanism. Nanoscale, 2020, 12, 18750-18760.	5.6	10
65	Using real space pseudopotentials for the electronic structure problem. Handbook of Numerical Analysis, 2003, 10, 613-637.	1.8	9
66	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
67	First-principles investigation of cubicBaRuO3: A Hund's metal. Physical Review B, 2016, 94, .	3.2	9
68	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
69	Thermodynamically stable octahedral MoS ₂ in van der Waals hetero-bilayers. 2D Materials, 2019, 6, 041002.	4.4	9
70	Oxygen Vacancyâ€Induced Topological Hall Effect in a Nonmagnetic Band Insulator. Advanced Quantum Technologies, 2020, 3, 2000021.	3.9	9
71	Native point defects in mono and bilayer phosphorene. Physical Review Materials, 2020, 4, .	2.4	9
72	Temperature-dependent layer breathing modes in two-dimensional materials. Physical Review B, 2018, 97, .	3.2	8

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73	Anisotropic Charge Transport in Nanoscale DNA Wire. Journal of Physical Chemistry C, 2020, 124, 16763-16772.	3.1	8
74	Density-Functional Theory of the Fractional Quantum Hall Effect. Physical Review Letters, 2017, 118, 196802.	7.8	7
75	Spontaneous Time-Reversal Symmetry Breaking at Individual Grain Boundaries in Graphene. Physical Review Letters, 2021, 126, 206803.	7.8	7
76	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
77	Electronic structure and spin polarization of MnGaP. Applied Physics Letters, 2004, 85, 2014-2016.	3.3	5
78	Structure of Iron-Containing Nitrogenated Carbon. Journal of Physical Chemistry C, 2008, 112, 9777-9782.	3.1	5
79	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></mm 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
80	Electrical and optical properties of low-bandgap oxide Zn2Mo3O8 for optoelectronic applications. Thin Solid Films, 2019, 677, 95-102.	1.8	5
81	Fine-tuning the DNA conductance by intercalation of drug molecules. Physical Review E, 2021, 103, 032411.	2.1	5
82	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
83	Molybdenum and Tungsten Di-sulfides: First Principles Investigation of Adatom Attachment and Diffusion on <i>c</i>-plane Alpha Sapphire and Correlation with Growth. Crystal Growth and Design, 2022, 22, 4708-4720.	3.0	4
84	Population analysis with Wannier orbitals. Journal of Chemical Physics, 2021, 154, 104111.	3.0	3
85	Tunable lattice thermal conductivity of twisted bilayer MoS₂. Physical Chemistry Chemical Physics, 2022, 24, 13860-13868.	2.8	3
86	Polarization discontinuity driven two dimensional electron gas at A2Mo3O8/B2Mo3O8 (A, B: Zn, Mg,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	2.5	2
87	Large intrinsic magnetization in an epitaxial BiFeO3/NdGaO3system. Europhysics Letters, 2019, 126, 57003.	2.0	1
88	Simulating Semiconductor Liquids with Ab Initio Pseudopotentials and Quantum Forces. Springer Proceedings in Physics, 2003, , 149-162.	0.2	1
89	Efficient hybrid and screened hybrid density functional calculations of carbon and silicon nanostructures electronic properties. , 2018, , .		0
90	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