

## List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

256 papers	43,760 citations	70 h-index	208 g-index
275 ext. papers	52,683 ext. citations	7.1 avg, IF	7.5 L-index

#	Paper	IF	Citations
256	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. <i>Journal of Physics Condensed Matter</i> , <b>2009</b> , 21, 395502	1.8	13251
255	Maximally localized generalized Wannier functions for composite energy bands. <i>Physical Review B</i> , <b>1997</b> , 56, 12847-12865	3.3	2886
254	Advanced capabilities for materials modelling with Quantum ESPRESSO. <i>Journal of Physics Condensed Matter</i> , <b>2017</b> , 29, 465901	1.8	2275
253	wannier90: A tool for obtaining maximally-localised Wannier functions. <i>Computer Physics Communications</i> , <b>2008</b> , 178, 685-699	4.2	2088
252	Maximally localized Wannier functions: Theory and applications. <i>Reviews of Modern Physics</i> , <b>2012</b> , 84, 1419-1475	40.5	1475
251	Uniaxial strain in graphene by Raman spectroscopy: G peak splitting, Grüneisen parameters, and sample orientation. <i>Physical Review B</i> , <b>2009</b> , 79,	3.3	1422
250	Maximally localized Wannier functions for entangled energy bands. <i>Physical Review B</i> , <b>2001</b> , 65,	3.3	1174
249	An updated version of wannier90: A tool for obtaining maximally-localised Wannier functions. <i>Computer Physics Communications</i> , <b>2014</b> , 185, 2309-2310	4.2	949
248	Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds. <i>Nature Nanotechnology</i> , <b>2018</b> , 13, 246-252	28.7	874
247	First-principles determination of the structural, vibrational and thermodynamic properties of diamond, graphite, and derivatives. <i>Physical Review B</i> , <b>2005</b> , 71,	3.3	823
246	Reproducibility in density functional theory calculations of solids. <i>Science</i> , <b>2016</b> , 351, aad3000	33.3	784
245	Thermal Contraction and Disorder of the Al(110) Surface. <i>Physical Review Letters</i> , <b>1999</b> , 82, 3296-3299	7.4	700
244	Large-Area Epitaxial Monolayer MoS <sub>2</sub> . <i>ACS Nano</i> , <b>2015</b> , 9, 4611-20	16.7	583
243	The shear mode of multilayer graphene. <i>Nature Materials</i> , <b>2012</b> , 11, 294-300	27	482
242	Density functional theory in transition-metal chemistry: a self-consistent Hubbard U approach. <i>Physical Review Letters</i> , <b>2006</b> , 97, 103001	7.4	421
241	Thermal conductivity of graphene and graphite: collective excitations and mean free paths. <i>Nano Letters</i> , <b>2014</b> , 14, 6109-14	11.5	353
240	Surface energies, work functions, and surface relaxations of low-index metallic surfaces from first principles. <i>Physical Review B</i> , <b>2009</b> , 80,	3.3	340

239	Role of disorder and anharmonicity in the thermal conductivity of silicon-germanium alloys: a first-principles study. <i>Physical Review Letters</i> , <b>2011</b> , 106, 045901	7.4	332
238	Phonon anharmonicities in graphite and graphene. <i>Physical Review Letters</i> , <b>2007</b> , 99, 176802	7.4	327
237	Maximally-localized Wannier functions for disordered systems: Application to amorphous silicon. <i>Solid State Communications</i> , <b>1998</b> , 107, 7-11	1.6	320
236	Revised self-consistent continuum solvation in electronic-structure calculations. <i>Journal of Chemical Physics</i> , <b>2012</b> , 136, 064102	3.9	293
235	Phonon hydrodynamics in two-dimensional materials. <i>Nature Communications</i> , <b>2015</b> , 6, 6400	17.4	282
234	Self-assembled quantum dots in a nanowire system for quantum photonics. <i>Nature Materials</i> , <b>2013</b> , 12, 439-44	27	278
233	Ensemble Density-Functional Theory for Ab Initio Molecular Dynamics of Metals and Finite-Temperature Insulators. <i>Physical Review Letters</i> , <b>1997</b> , 79, 1337-1340	7.4	277
232	AiiDA: automated interactive infrastructure and database for computational science. <i>Computational Materials Science</i> , <b>2016</b> , 111, 218-230	3.2	275
231	Electrochemical Windows of Room-Temperature Ionic Liquids from Molecular Dynamics and Density Functional Theory Calculations. <i>Chemistry of Materials</i> , <b>2011</b> , 23, 2979-2986	9.6	271
230	Surface composition tuning of Au-Pt bimetallic nanoparticles for enhanced carbon monoxide and methanol electro-oxidation. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 7985-91	16.4	240
229	Wannier90 as a community code: new features and applications. <i>Journal of Physics Condensed Matter</i> , <b>2020</b> , 32, 165902	1.8	239
228	Exponential localization of Wannier functions in insulators. <i>Physical Review Letters</i> , <b>2007</b> , 98, 046402	7.4	235
227	Quantum ESPRESSO toward the exascale. <i>Journal of Chemical Physics</i> , <b>2020</b> , 152, 154105	3.9	227
226	Performance of arsenene and antimonene double-gate MOSFETs from first principles. <i>Nature Communications</i> , <b>2016</b> , 7, 12585	17.4	224
225	Ab initio transport properties of nanostructures from maximally localized Wannier functions. <i>Physical Review B</i> , <b>2004</b> , 69,	3.3	220
224	Ultraviolet Photodetectors Based on Anodic TiO <sub>2</sub> Nanotube Arrays. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 10725-10729	3.8	206
223	Oxygen Evolution Reaction on La <sub>1-x</sub> Sr <sub>x</sub> CoO <sub>3</sub> Perovskites: A Combined Experimental and Theoretical Study of Their Structural, Electronic, and Electrochemical Properties. <i>Chemistry of Materials</i> , <b>2015</b> , 27, 7662-7672	9.6	200
222	Static dielectric properties of carbon nanotubes from first principles. <i>Physical Review Letters</i> , <b>2006</b> , 96, 166801	7.4	195

221	Sensing mechanisms for carbon nanotube based NH <sub>3</sub> gas detection. <i>Nano Letters</i> , <b>2009</b> , 9, 1626-30	11.5	191
220	Precision and efficiency in solid-state pseudopotential calculations. <i>Npj Computational Materials</i> , <b>2018</b> , 4,	10.9	181
219	Production and processing of graphene and related materials. <i>2D Materials</i> , <b>2020</b> , 7, 022001	5.9	179
218	Static and dynamical properties of heavy water at ambient conditions from first-principles molecular dynamics. <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 204510	3.9	177
217	Koopmans condition for density-functional theory. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	176
216	BoltzWann: A code for the evaluation of thermoelectric and electronic transport properties with a maximally-localized Wannier functions basis. <i>Computer Physics Communications</i> , <b>2014</b> , 185, 422-429	4.2	166
215	Potential-induced nanoclustering of metallic catalysts during electrochemical CO reduction. <i>Nature Communications</i> , <b>2018</b> , 9, 3117	17.4	163
214	Predicting synthesizability. <i>Journal Physics D: Applied Physics</i> , <b>2019</b> , 52,	3	161
213	Acoustic phonon lifetimes and thermal transport in free-standing and strained graphene. <i>Nano Letters</i> , <b>2012</b> , 12, 2673-8	11.5	154
212	Band structure and quantum conductance of nanostructures from maximally localized Wannier functions: the case of functionalized carbon nanotubes. <i>Physical Review Letters</i> , <b>2005</b> , 95, 076804	7.4	152
211	Simulation of heme using DFT + U: a step toward accurate spin-state energetics. <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 7384-91	3.4	122
210	Highly Active and Stable Iridium Pyrochlores for Oxygen Evolution Reaction. <i>Chemistry of Materials</i> , <b>2017</b> , 29, 5182-5191	9.6	120
209	Achieving DFT accuracy with a machine-learning interatomic potential: Thermomechanics and defects in bcc ferromagnetic iron. <i>Physical Review Materials</i> , <b>2018</b> , 2,	3.2	115
208	Electron-phonon interactions and the intrinsic electrical resistivity of graphene. <i>Nano Letters</i> , <b>2014</b> , 14, 1113-9	11.5	109
207	Cycloaddition functionalizations to preserve or control the conductance of carbon nanotubes. <i>Physical Review Letters</i> , <b>2006</b> , 97, 116801	7.4	108
206	A unified electrostatic and cavitation model for first-principles molecular dynamics in solution. <i>Journal of Chemical Physics</i> , <b>2006</b> , 124, 74103	3.9	101
205	Electrostatics in periodic boundary conditions and real-space corrections. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	99
204	The role of nanostructure in the wetting behavior of mixed-monolayer-protected metal nanoparticles. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2008</b> , 105, 9886-91	11.5	98

203	Band-like electron transport with record-high mobility in the TCNQ family. <i>Advanced Materials</i> , <b>2015</b> , 27, 2453-8	24	97
202	Unified theory of thermal transport in crystals and glasses. <i>Nature Physics</i> , <b>2019</b> , 15, 809-813	16.2	94
201	The Electronic Thermal Conductivity of Graphene. <i>Nano Letters</i> , <b>2016</b> , 16, 2439-43	11.5	92
200	Spin channels in functionalized graphene nanoribbons. <i>Nano Letters</i> , <b>2009</b> , 9, 3425-9	11.5	91
199	Photoinduced oxidation of carbon nanotubes. <i>Journal of Physics Condensed Matter</i> , <b>2003</b> , 15, 5915-5921	11.8	87
198	Breakdown of Optical Phonons' Splitting in Two-Dimensional Materials. <i>Nano Letters</i> , <b>2017</b> , 17, 3758-3763	11.5	84
197	Grand canonical simulations of electrochemical interfaces in implicit solvation models. <i>Journal of Chemical Physics</i> , <b>2019</b> , 150, 041730	3.9	80
196	An In Situ Surface-Enhanced Infrared Absorption Spectroscopy Study of Electrochemical CO <sub>2</sub> Reduction: Selectivity Dependence on Surface C-Bound and O-Bound Reaction Intermediates. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 5951-5963	3.8	78
195	Hubbard parameters from density-functional perturbation theory. <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	77
194	Spatially extended Kondo state in magnetic molecules induced by interfacial charge transfer. <i>Physical Review Letters</i> , <b>2010</b> , 105, 106601	7.4	77
193	Phonon-limited resistivity of graphene by first-principles calculations: Electron-phonon interactions, strain-induced gauge field, and Boltzmann equation. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	76
192	Defect ordering and defect-domain-wall interactions in PbTiO <sub>3</sub> : A first-principles study. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	75
191	High thermal conductivity in short-period superlattices. <i>Nano Letters</i> , <b>2011</b> , 11, 5135-41	11.5	75
190	Unraveling Thermodynamics, Stability, and Oxygen Evolution Activity of Strontium Ruthenium Perovskite Oxide. <i>ACS Catalysis</i> , <b>2017</b> , 7, 3245-3256	13.1	74
189	Self-consistent continuum solvation (SCCS): the case of charged systems. <i>Journal of Chemical Physics</i> , <b>2013</b> , 139, 214110	3.9	73
188	Systematic study of first-row transition-metal diatomic molecules: a self-consistent DFT+U approach. <i>Journal of Chemical Physics</i> , <b>2010</b> , 133, 114103	3.9	73
187	Equipartition of Energy Defines the Size-Thickness Relationship in Liquid-Exfoliated Nanosheets. <i>ACS Nano</i> , <b>2019</b> , 13, 7050-7061	16.7	71
186	Materials Cloud, a platform for open computational science. <i>Scientific Data</i> , <b>2020</b> , 7, 299	8.2	70

185	pi-Stacking in thiophene oligomers as the driving force for electroactive materials and devices. <i>Journal of the American Chemical Society</i> , <b>2005</b> , 127, 3207-12	16.4	69
184	A generalized Poisson and Poisson-Boltzmann solver for electrostatic environments. <i>Journal of Chemical Physics</i> , <b>2016</b> , 144, 014103	3.9	69
183	Proton dynamics in superprotonic CsHSO <sub>4</sub> . <i>Physical Review B</i> , <b>2007</b> , 76,	3.3	67
182	Sliding Mechanisms in Aluminum Grain Boundaries. <i>Physical Review Letters</i> , <b>1997</b> , 79, 869-872	7.4	65
181	Soft-Sphere Continuum Solvation in Electronic-Structure Calculations. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 3829-3845	6.4	64
180	Emergence of One-Dimensional Wires of Free Carriers in Transition-Metal-Dichalcogenide Nanostructures. <i>Nano Letters</i> , <b>2015</b> , 15, 6229-38	11.5	64
179	Berry phase and pseudospin winding number in bilayer graphene. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	64
178	Koopmans-compliant functionals and their performance against reference molecular data. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	63
177	A self-consistent Hubbard U density-functional theory approach to the addition-elimination reactions of hydrocarbons on bare FeO <sup>+</sup> . <i>Journal of Chemical Physics</i> , <b>2008</b> , 129, 134314	3.9	61
176	Electrostatics of solvated systems in periodic boundary conditions. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	60
175	Effects of filling in CoSb <sub>3</sub> : Local structure, band gap, and phonons from first principles. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	60
174	Large-scale synthesis of crystalline g-CN nanosheets and high-temperature H sieving from assembled films. <i>Science Advances</i> , <b>2020</b> , 6, eaay9851	14.3	59
173	Ionic correlations and failure of Nernst-Einstein relation in solid-state electrolytes. <i>Physical Review Materials</i> , <b>2017</b> , 1,	3.2	58
172	Accurate potential energy surfaces with a DFT+U(R) approach. <i>Journal of Chemical Physics</i> , <b>2011</b> , 135, 194105	3.9	56
171	Structure and phase stability of Ga <sub>x</sub> In <sub>1-x</sub> P solid solutions from computational alchemy. <i>Physical Review Letters</i> , <b>1994</b> , 72, 4001-4004	7.4	56
170	π-Stacking in Charged Thiophene Oligomers. <i>Journal of Physical Chemistry B</i> , <b>2004</b> , 108, 17791-17795	3.4	55
169	Dielectric response of oxides in the weighted density approximation. <i>Physical Review B</i> , <b>2000</b> , 62, 12724-12729	3.3	55
168	Thermal Transport in Crystals as a Kinetic Theory of Relaxons. <i>Physical Review X</i> , <b>2016</b> , 6,	9.1	53

167	Improving the electrical conductivity of carbon nanotube networks: a first-principles study. <i>ACS Nano</i> , <b>2011</b> , 5, 9726-36	16.7	53
166	Realistic quantitative descriptions of electron transfer reactions: diabatic free-energy surfaces from first-principles molecular dynamics. <i>Physical Review Letters</i> , <b>2006</b> , 97, 028303	7.4	53
165	Mobility of two-dimensional materials from first principles in an accurate and automated framework. <i>Physical Review Materials</i> , <b>2018</b> , 2,	3.2	51
164	First-principles prediction of the equilibrium shape of nanoparticles under realistic electrochemical conditions. <i>Physical Review Letters</i> , <b>2013</b> , 110, 086104	7.4	50
163	A converse approach to the calculation of NMR shielding tensors. <i>Journal of Chemical Physics</i> , <b>2009</b> , 131, 101101	3.9	49
162	AiiDA 1.0, a scalable computational infrastructure for automated reproducible workflows and data provenance. <i>Scientific Data</i> , <b>2020</b> , 7, 300	8.2	49
161	Playing quantum hide-and-seek with the muon: localizing muon stopping sites. <i>Physica Scripta</i> , <b>2013</b> , 88, 068510	2.6	48
160	Spin and orbital magnetic response in metals: Susceptibility and NMR shifts. <i>Physical Review B</i> , <b>2007</b> , 76,	3.3	47
159	Prediction of a Large-Gap and Switchable Kane-Mele Quantum Spin Hall Insulator. <i>Physical Review Letters</i> , <b>2018</b> , 120, 117701	7.4	45
158	Textural and Micromorphological Effects on the Overall Elastic Response of Macroscopically Anisotropic Composites. <i>Journal of Applied Mechanics, Transactions ASME</i> , <b>1992</b> , 59, 269-275	2.7	45
157	Insight into gallium behavior in aluminum grain boundaries from calculation on $\Sigma 11$ (113) boundary. <i>Acta Materialia</i> , <b>2000</b> , 48, 3623-3632	8.4	44
156	Transition-metal dioxides: a case for the intersite term in Hubbard-model functionals. <i>Journal of Chemical Physics</i> , <b>2011</b> , 134, 094103	3.9	43
155	First-principles study of non-heme Fe(II) halogenase SyrB2 reactivity. <i>Journal of the American Chemical Society</i> , <b>2009</b> , 131, 14426-33	16.4	43
154	Continuum models of the electrochemical diffuse layer in electronic-structure calculations. <i>Journal of Chemical Physics</i> , <b>2019</b> , 150, 041722	3.9	43
153	Hydrogen bonding and coordination in normal and supercritical water from x-ray inelastic scattering. <i>Physical Review B</i> , <b>2007</b> , 76,	3.3	42
152	High-throughput computational screening for solid-state Li-ion conductors. <i>Energy and Environmental Science</i> , <b>2020</b> , 13, 928-948	35.4	42
151	Highly Active Nanoperovskite Catalysts for Oxygen Evolution Reaction: Insights into Activity and Stability of $\text{Ba}_{0.5}\text{Sr}_{0.5}\text{Co}_{0.8}\text{Fe}_{0.2}\text{O}_{2+\delta}$ and $\text{PrBaCo}_2\text{O}_{5+\delta}$ <i>Advanced Functional Materials</i> , <b>2018</b> , 28, 1804355	15.6	41
150	An Open-Source Multiscale Framework for the Simulation of Nanoscale Devices. <i>IEEE Transactions on Electron Devices</i> , <b>2014</b> , 61, 48-53	2.9	40



149	Electronic-enthalpy functional for finite systems under pressure. <i>Physical Review Letters</i> , <b>2005</b> , 94, 145501	14	40
148	Local effects in the X-ray absorption spectrum of salt water. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 9594-601	3.4	38
147	Gate modulation in carbon nanotube field effect transistors-based NH <sub>3</sub> gas sensors. <i>Sensors and Actuators B: Chemical</i> , <b>2008</b> , 132, 191-195	8.5	38
146	Engineering polar discontinuities in honeycomb lattices. <i>Nature Communications</i> , <b>2014</b> , 5, 5157	17.4	37
145	Quantum states of muons in fluorides. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	37
144	Evidence of Large Polarons in Photoemission Band Mapping of the Perovskite Semiconductor CsPbBr <sub>3</sub> . <i>Physical Review Letters</i> , <b>2020</b> , 124, 206402	7.4	36
143	Vibrational recognition of adsorption sites for CO on platinum and platinum-ruthenium surfaces. <i>Journal of the American Chemical Society</i> , <b>2007</b> , 129, 11045-52	16.4	36
142	NMR shifts for polycyclic aromatic hydrocarbons from first-principles. <i>International Journal of Quantum Chemistry</i> , <b>2009</b> , 109, 3336-3342	2.1	34
141	First principles calculation of the energy and structure of two solid surface phases on Ir{100}. <i>Surface Science</i> , <b>1998</b> , 418, 529-535	1.8	34
140	Screw dislocation structure and mobility in body centered cubic Fe predicted by a Gaussian Approximation Potential. <i>Npj Computational Materials</i> , <b>2018</b> , 4,	10.9	34
139	Solvent-Aware Interfaces in Continuum Solvation. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 1996-2009	6.4	33
138	First-principles photoemission spectroscopy and orbital tomography in molecules from koopmans-compliant functionals. <i>Physical Review Letters</i> , <b>2015</b> , 114, 166405	7.4	33
137	Absolute band alignment at semiconductor-water interfaces using explicit and implicit descriptions for liquid water. <i>Npj Computational Materials</i> , <b>2019</b> , 5,	10.9	33
136	Donor and acceptor levels of organic photovoltaic compounds from first principles. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 685-95	3.6	33
135	A classical and ab initio study of the interaction of the myosin triphosphate binding domain with ATP. <i>Biophysical Journal</i> , <b>2002</b> , 82, 660-75	2.9	33
134	Photoelectron properties of DNA and RNA bases from many-body perturbation theory. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	32
133	Transport properties of room-temperature ionic liquids from classical molecular dynamics. <i>Journal of Chemical Physics</i> , <b>2012</b> , 137, 044508	3.9	32
132	Bulk aluminum at high pressure: A first-principles study. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	32



131	Materials modelling: The frontiers and the challenges. <i>Nature Materials</i> , <b>2016</b> , 15, 381-2	27	31
130	Dominant phonon wave vectors and strain-induced splitting of the 2D Raman mode of graphene. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	31
129	Unique carbon-nanotube field-effect transistors with asymmetric source and drain contacts. <i>Nano Letters</i> , <b>2008</b> , 8, 64-8	11.5	31
128	Boltzmann Transport in Nanostructures as a Friction Effect. <i>Nano Letters</i> , <b>2017</b> , 17, 4675-4682	11.5	30
127	Thermoelastic properties of Iron from first-principles. <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	29
126	Spin-resolved optical conductivity of two-dimensional group-VIB transition-metal dichalcogenides. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	29
125	Maximally localized Wannier functions in antiferromagnetic MnO within the FLAPW formalism. <i>Physical Review B</i> , <b>2002</b> , 65,	3.3	29
124	Relative Abundance of [Formula: see text] Topological Order in Exfoliable Two-Dimensional Insulators. <i>Nano Letters</i> , <b>2019</b> , 19, 8431-8440	11.5	27
123	Enhanced Proton Conductivity in Y-Doped BaZrO via Strain Engineering. <i>Advanced Science</i> , <b>2017</b> , 4, 1700467	11.5	27
122	Thermodynamic stability of alkali-metal/zinc double-cation borohydrides at low temperatures. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	27
121	Rippling ultrafast dynamics of suspended 2D monolayers, graphene. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2016</b> , 113, E6555-E6561	11.5	27
120	Bridging density-functional and many-body perturbation theory: Orbital-density dependence in electronic-structure functionals. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	26
119	Enhanced Electron-Phonon Interaction in Multivalley Materials. <i>Physical Review X</i> , <b>2019</b> , 9,	9.1	25
118	Dynamical structure, bonding, and thermodynamics of the superionic sublattice in alpha-Agl. <i>Physical Review Letters</i> , <b>2006</b> , 97, 166401	7.4	25
117	Electrosorption at metal surfaces from first principles. <i>Npj Computational Materials</i> , <b>2020</b> , 6,	10.9	25
116	Nanoscale surface dynamics of BiTe(111): observation of a prominent surface acoustic wave and the role of van der Waals interactions. <i>Nanoscale</i> , <b>2018</b> , 10, 14627-14636	7.7	24
115	Conductance Switching and Many-Valued Logic in Porphyrin Assemblies. <i>Journal of Physical Chemistry Letters</i> , <b>2013</b> , 4, 3039-3044	6.4	24
114	Automated quantum conductance calculations using maximally-localised Wannier functions. <i>Computer Physics Communications</i> , <b>2011</b> , 182, 2174-2183	4.2	24

113	Lattice anharmonicity in low-dimensional carbon systems. <i>Physica Status Solidi (B): Basic Research</i> , <b>2008</b> , 245, 2149-2154	1.3	24
112	Electronic-structure methods for materials design. <i>Nature Materials</i> , <b>2021</b> , 20, 736-749	27	24
111	Modeling lithium-ion solid-state electrolytes with a pinball model. <i>Physical Review Materials</i> , <b>2018</b> , 2,	3.2	23
110	Variational minimization of orbital-density-dependent functionals. <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	22
109	Electronic, vibrational, and transport properties of pnictogen-substituted ternary skutterudites. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	22
108	Ab initio converse NMR approach for pseudopotentials. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	22
107	Dielectric response of periodic systems from quantum Monte Carlo calculations. <i>Physical Review Letters</i> , <b>2005</b> , 95, 207602	7.4	22
106	Self-consistent site-dependent DFT+U study of stoichiometric and defective SrMnO <sub>3</sub> . <i>Physical Review B</i> , <b>2019</b> , 99,	3.3	21
105	Chemisorbed Molecules under Potential Bias: Detailed Insights from First-Principles Vibrational Spectroscopies. <i>Electrochimica Acta</i> , <b>2014</b> , 121, 210-214	6.7	21
104	First-principles characterization of the structure and electronic structure of B and Rh-S chalcogenides. <i>Physical Review B</i> , <b>2009</b> , 80,	3.3	21
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