Nicola Marzari

List of Publications by Year in Descending Order

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	Structure Evolution of Graphitic Surface upon Oxidation: Insights by Scanning Tunneling Microscopy.. *Jacs Au*, **2022**, 2, 723-730		1
255	Phonon-Assisted Luminescence in Defect Centers from Many-Body Perturbation Theory.. *Physical Review Letters*, **2022**, 128, 167401	7.4	3
254	First-principles predictions of Hall and drift mobilities in semiconductors. *Physical Review Research*, **2021**, 3,	3.9	5
253	Thermomechanical properties of honeycomb lattices from internal-coordinates potentials: the case of graphene and hexagonal boron nitride. *2D Materials*, **2021**, 8, 015026	5.9	2
252	High Li-ion conductivity in tetragonal LGPO: A comparative first-principles study against known LISICON and LGPS phases. *Physical Review Materials*, **2021**, 5,	3.2	2
251	Prediction of Phonon-Mediated Superconductivity with High Critical Temperature in the Two-Dimensional Topological Semimetal WN. *Nano Letters*, **2021**, 21, 3435-3442	11.5	8
250	Theoretical Prediction of Two-Dimensional Materials, Behavior, and Properties. *ACS Nano*, **2021**, 15, 5959-5976	16.7	68
249	Electronic-structure methods for materials design. *Nature Materials*, **2021**, 20, 736-749	27	24
248	Electronic Structure of Water from Koopmans-Compliant Functionals. *Journal of Chemical Theory and Computation*, **2021**, 17, 3923-3930	6.4	0
247	Workflows in AiiDA: Engineering a high-throughput, event-based engine for robust and modular computational workflows. *Computational Materials Science*, **2021**, 187, 110086	3.2	18
246	Self-consistent Hubbard parameters from density-functional perturbation theory in the ultrasoft and projector-augmented wave formulations. *Physical Review B*, **2021**, 103,	3.3	14
245	AiiDAlab an ecosystem for developing, executing, and sharing scientific workflows. *Computational Materials Science*, **2021**, 188, 110165	3.2	18
244	OPTIMADE, an API for exchanging materials data. *Scientific Data*, **2021**, 8, 217	8.2	8
243	Shear and Breathing Modes of Layered Materials. *ACS Nano*, **2021**,	16.7	4
242	Gas Transport across Carbon Nitride Nanopores: A Comparison of van der Waals Functionals against the Random-Phase Approximation. *Journal of Physical Chemistry C*, **2021**, 125, 18896-18904	3.8	0
241	Common workflows for computing material properties using different quantum engines. *Npj Computational Materials*, **2021**, 7,	10.9	4
240	Gate Control of Spin-Layer-Locking FETs and Application to Monolayer LuIO. *Nano Letters*, **2021**, 21, 7631-7636	11.5	1

239	Ab initio Electron-Phonon Interactions in Correlated Electron Systems. *Physical Review Letters*, **2021**, 127, 126404	7.4	3
238	Evidence of Large Polarons in Photoemission Band Mapping of the Perovskite Semiconductor CsPbBr_{3}. *Physical Review Letters*, **2020**, 124, 206402	7.4	36
237	The solid-state Li-ion conductor Li7TaO6: A combined computational and experimental study. *Solid State Ionics*, **2020**, 347, 115226	3.3	3
236	2-D Materials for Ultrascaled Field-Effect Transistors: One Hundred Candidates under the Microscope. *ACS Nano*, **2020**, 14, 8605-8615	16.7	20
235	Bulk and Surface Electronic Structure of the Dual-Topology Semimetal Pt_{2}HgSe_{3}. *Physical Review Letters*, **2020**, 124, 106402	7.4	20
234	Hubbard-corrected density functional perturbation theory with ultrasoft pseudopotentials. *Physical Review B*, **2020**, 101,	3.3	14
233	Production and processing of graphene and related materials. *2D Materials*, **2020**, 7, 022001	5.9	179
232	Large-scale synthesis of crystalline g-CN nanosheets and high-temperature H sieving from assembled films. *Science Advances*, **2020**, 6, eaay9851	14.3	59
231	Generalization of Fourier's Law into Viscous Heat Equations. *Physical Review X*, **2020**, 10,	9.1	16
230	Intrinsic edge excitons in two-dimensional MoS2. *Physical Review B*, **2020**, 101,	3.3	2
229	Pulay forces in density-functional theory with extended Hubbard functionals: From nonorthogonalized to orthogonalized manifolds. *Physical Review B*, **2020**, 102,	3.3	4
228	Emergent dual topology in the three-dimensional Kane-Mele Pt2HgSe3. *Physical Review Research*, **2020**, 2,	3.9	11
227	Self-consistent DFT+U+V study of oxygen vacancies in SrTiO3. *Physical Review Research*, **2020**, 2,	3.9	16
226	Electronic structure of pristine and Ni-substituted LaFeO3 from near edge x-ray absorption fine structure experiments and first-principles simulations. *Physical Review Research*, **2020**, 2,	3.9	7
225	On the Kinetic Theory of Thermal Transport in Crystals **2020**, 767-808		
224	Operando XANES from first-principles and its application to iridium oxide. *Physical Chemistry Chemical Physics*, **2020**, 22, 10807-10818	3.6	10
223	Wannier90 as a community code: new features and applications. *Journal of Physics Condensed Matter*, **2020**, 32, 165902	1.8	239
222	High-throughput computational screening for solid-state Li-ion conductors. *Energy and Environmental Science*, **2020**, 13, 928-948	35.4	42

221	Role of OH Intermediates during the Au Oxide Electro-Reduction at Low pH Elucidated by Electrochemical Surface-Enhanced Raman Spectroscopy and Implicit Solvent Density Functional Theory. *ACS Catalysis*, **2020**, 10, 12716-12726	13.1	6
220	Automated high-throughput Wannierisation. *Npj Computational Materials*, **2020**, 6,	10.9	15
219	Efficient Kr/Xe separation from triangular g-C3N4 nanopores, a simulation study. *Journal of Materials Chemistry A*, **2020**, 8, 17747-17755	13	3
218	Electrosorption at metal surfaces from first principles. *Npj Computational Materials*, **2020**, 6,	10.9	25
217	AiiDA 1.0, a scalable computational infrastructure for automated reproducible workflows and data provenance. *Scientific Data*, **2020**, 7, 300	8.2	49
216	Materials Cloud, a platform for open computational science. *Scientific Data*, **2020**, 7, 299	8.2	70
215	Li4□Ge1□PxO4, a Potential Solid-State Electrolyte for All-Oxide Microbatteries. *ACS Applied Energy Materials*, **2020**, 3, 9910-9917	6.1	4
214	Quantum ESPRESSO toward the exascale. *Journal of Chemical Physics*, **2020**, 152, 154105	3.9	227
213	Yttrium Tantalum Oxynitride Multiphases as Photoanodes for Water Oxidation. *Journal of Physical Chemistry C*, **2019**, 123, 26211-26217	3.8	7
212	Solvent-Aware Interfaces in Continuum Solvation. *Journal of Chemical Theory and Computation*, **2019**, 15, 1996-2009	6.4	33
211	Grand canonical simulations of electrochemical interfaces in implicit solvation models. *Journal of Chemical Physics*, **2019**, 150, 041730	3.9	80
210	Unified theory of thermal transport in crystals and glasses. *Nature Physics*, **2019**, 15, 809-813	16.2	94
209	Equipartition of Energy Defines the Size-Thickness Relationship in Liquid-Exfoliated Nanosheets. *ACS Nano*, **2019**, 13, 7050-7061	16.7	71
208	Valley-Engineering Mobilities in Two-Dimensional Materials. *Nano Letters*, **2019**, 19, 3723-3729	11.5	10
207	Koopmans Meets Bethe-Salpeter: Excitonic Optical Spectra without GW. *Journal of Chemical Theory and Computation*, **2019**, 15, 3710-3720	6.4	9
206	Self-consistent site-dependent DFT+U study of stoichiometric and defective SrMnO3. *Physical Review B*, **2019**, 99,	3.3	21
205	SIMPLE code: Optical properties with optimal basis functions. *Computer Physics Communications*, **2019**, 240, 106-119	4.2	11
204	Predicting synthesizability. *Journal Physics D: Applied Physics*, **2019**, 52,	3	161

203	Enhanced Electron-Phonon Interaction in Multivalley Materials. *Physical Review X*, **2019**, 9,	9.1	25
202	Functional Extrapolations to Tame Unbound Anions in Density-Functional Theory Calculations. *Journal of Chemical Theory and Computation*, **2019**, 15, 6313-6322	6.4	5
201	Absolute band alignment at semiconductor-water interfaces using explicit and implicit descriptions for liquid water. *Npj Computational Materials*, **2019**, 5,	10.9	33
200	A High-Throughput Computational Study Driven by the AiiDA Materials Informatics Framework and the PAULING FILE as Reference Database **2019**, 149-170		1
199	Relative Abundance of [Formula: see text] Topological Order in Exfoliable Two-Dimensional Insulators. *Nano Letters*, **2019**, 19, 8431-8440	11.5	27
198	Energetics and cathode voltages of LiMPO4 olivines (M=Fe, Mn) from extended Hubbard functionals. *Physical Review Materials*, **2019**, 3,	3.2	19
197	Unsupervised landmark analysis for jump detection in molecular dynamics simulations. *Physical Review Materials*, **2019**, 3,	3.2	17
196	Photorealistic modelling of metals from first principles. *Npj Computational Materials*, **2019**, 5,	10.9	10
195	Halogen-bond driven self-assembly of perfluorocarbon monolayers on silicon nitride. *Journal of Materials Chemistry A*, **2019**, 7, 24445-24453	13	6
194	An In Situ Surface-Enhanced Infrared Absorption Spectroscopy Study of Electrochemical CO2 Reduction: Selectivity Dependence on Surface C-Bound and O-Bound Reaction Intermediates. *Journal of Physical Chemistry C*, **2019**, 123, 5951-5963	3.8	78
193	Continuum models of the electrochemical diffuse layer in electronic-structure calculations. *Journal of Chemical Physics*, **2019**, 150, 041722	3.9	43
192	Koopmans-Compliant Functionals and Potentials and Their Application to the GW100 Test Set. *Journal of Chemical Theory and Computation*, **2019**, 15, 1905-1914	6.4	15
191	Screening in Orbital-Density-Dependent Functionals. *Journal of Chemical Theory and Computation*, **2018**, 14, 2549-2557	6.4	8
190	Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds. *Nature Nanotechnology*, **2018**, 13, 246-252	28.7	874
189	Prediction of a Large-Gap and Switchable Kane-Mele Quantum Spin Hall Insulator. *Physical Review Letters*, **2018**, 120, 117701	7.4	45
188	Nanoscale surface dynamics of BiTe(111): observation of a prominent surface acoustic wave and the role of van der Waals interactions. *Nanoscale*, **2018**, 10, 14627-14636	7.7	24
187	Hubbard parameters from density-functional perturbation theory. *Physical Review B*, **2018**, 98,	3.3	77
186	Potential-induced nanoclustering of metallic catalysts during electrochemical CO reduction. *Nature Communications*, **2018**, 9, 3117	17.4	163

185	. *IEEE Transactions on Electron Devices*, **2018**, 65, 4180-4187	2.9	15
184	Achieving DFT accuracy with a machine-learning interatomic potential: Thermomechanics and defects in bcc ferromagnetic iron. *Physical Review Materials*, **2018**, 2,	3.2	115
183	Modeling lithium-ion solid-state electrolytes with a pinball model. *Physical Review Materials*, **2018**, 2,	3.2	23
182	Mobility of two-dimensional materials from first principles in an accurate and automated framework. *Physical Review Materials*, **2018**, 2,	3.2	51
181	Precision and efficiency in solid-state pseudopotential calculations. *Npj Computational Materials*, **2018**, 4,	10.9	181
180	Screw dislocation structure and mobility in body centered cubic Fe predicted by a Gaussian Approximation Potential. *Npj Computational Materials*, **2018**, 4,	10.9	34
179	Highly Active Nanoperovskite Catalysts for Oxygen Evolution Reaction: Insights into Activity and Stability of Ba0.5Sr0.5Co0.8Fe0.2O2+□and PrBaCo2O5+□*Advanced Functional Materials*, **2018**, 28, 1804355	15.6	41
178	On the Kinetic Theory of Thermal Transport in Crystals **2018**, 1-42		
177	Koopmans-Compliant Spectral Functionals for Extended Systems. *Physical Review X*, **2018**, 8,	9.1	18
176	Vibrational and thermoelastic properties of bcc iron from selected EAM potentials. *Computational Materials Science*, **2018**, 152, 99-106	3.2	4
175	Piezoelectric softening by Nb substitution in (Ba,Pb)ZrO3 ceramics. *Journal of the American Ceramic Society*, **2017**, 100, 1885-1895	3.8	3
174	Breakdown of Optical Phonons' Splitting in Two-Dimensional Materials. *Nano Letters*, **2017**, 17, 3758-3763	11.5	84
173	Soft-Sphere Continuum Solvation in Electronic-Structure Calculations. *Journal of Chemical Theory and Computation*, **2017**, 13, 3829-3845	6.4	64
172	Highly Active and Stable Iridium Pyrochlores for Oxygen Evolution Reaction. *Chemistry of Materials*, **2017**, 29, 5182-5191	9.6	120
171	Determination of Conduction and Valence Band Electronic Structure of LaTiO N Thin Film. *ChemSusChem*, **2017**, 10, 2099-2106	8.3	13
170	Unraveling Thermodynamics, Stability, and Oxygen Evolution Activity of Strontium Ruthenium Perovskite Oxide. *ACS Catalysis*, **2017**, 7, 3245-3256	13.1	74
169	Advanced capabilities for materials modelling with Quantum ESPRESSO. *Journal of Physics Condensed Matter*, **2017**, 29, 465901	1.8	2275
168	Boltzmann Transport in Nanostructures as a Friction Effect. *Nano Letters*, **2017**, 17, 4675-4682	11.5	30

167	Enhanced Proton Conductivity in Y-Doped BaZrO via Strain Engineering. *Advanced Science*, **2017**, 4, 1700467	4.6	27
166	A posteriori metadata from automated provenance tracking: integration of AiiDA and TCOD. *Journal of Cheminformatics*, **2017**, 9, 56	8.6	15
165	Ionic correlations and failure of Nernst-Einstein relation in solid-state electrolytes. *Physical Review Materials*, **2017**, 1,	3.2	58
164	Transport waves as crystal excitations. *Physical Review Materials*, **2017**, 1,	3.2	14
163	Asymmetric structure of 90? domain walls and interactions with defects in PbTiO3. *Physical Review B*, **2016**, 93,	3.3	17
162	Thermal Transport in Crystals as a Kinetic Theory of Relaxons. *Physical Review X*, **2016**, 6,	9.1	53
161	Performance of arsenene and antimonene double-gate MOSFETs from first principles. *Nature Communications*, **2016**, 7, 12585	17.4	224
160	First-Principles Photoemission Spectroscopy of DNA and RNA Nucleobases from Koopmans-Compliant Functionals. *Journal of Chemical Theory and Computation*, **2016**, 12, 3948-58	6.4	9
159	Reproducibility in density functional theory calculations of solids. *Science*, **2016**, 351, aad3000	33.3	784
158	Materials modelling: The frontiers and the challenges. *Nature Materials*, **2016**, 15, 381-2	27	31
157	The Electronic Thermal Conductivity of Graphene. *Nano Letters*, **2016**, 16, 2439-43	11.5	92
156	AiiDA: automated interactive infrastructure and database for computational science. *Computational Materials Science*, **2016**, 111, 218-230	3.2	275
155	A generalized Poisson and Poisson-Boltzmann solver for electrostatic environments. *Journal of Chemical Physics*, **2016**, 144, 014103	3.9	69
154	First-principles molecular dynamics simulations of proton diffusion in cubic BaZrO(_3) perovskite under strain conditions. *Materials for Renewable and Sustainable Energy*, **2016**, 5, 1	4.7	7
153	Rippling ultrafast dynamics of suspended 2D monolayers, graphene. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, E6555-E6561	11.5	27
152	Phonon hydrodynamics in two-dimensional materials. *Nature Communications*, **2015**, 6, 6400	17.4	282
151	Thermoelastic properties of □ron from first-principles. *Physical Review B*, **2015**, 91,	3.3	29
150	Band-like electron transport with record-high mobility in the TCNQ family. *Advanced Materials*, **2015**, 27, 2453-8	24	97

149	Self-consistent continuum solvation for optical absorption of complex molecular systems in solution. *Journal of Chemical Physics*, **2015**, 142, 034111	3.9	14
148	First-principles investigation of organic photovoltaic materials C60, C70, [C60]PCBM, and bis-[C60]PCBM using a many-body G0W0-Lanczos approach. *Physical Review B*, **2015**, 91,	3.3	17
147	Variational minimization of orbital-density-dependent functionals. *Physical Review B*, **2015**, 91,	3.3	22
146	First-principles photoemission spectroscopy and orbital tomography in molecules from koopmans-compliant functionals. *Physical Review Letters*, **2015**, 114, 166405	7.4	33
145	Large-Area Epitaxial Monolayer MoS2. *ACS Nano*, **2015**, 9, 4611-20	16.7	583
144	Oxygen Evolution Reaction on La1SrxCoO3 Perovskites: A Combined Experimental and Theoretical Study of Their Structural, Electronic, and Electrochemical Properties. *Chemistry of Materials*, **2015**, 27, 7662-7672	9.6	200
143	Emergence of One-Dimensional Wires of Free Carriers in Transition-Metal-Dichalcogenide Nanostructures. *Nano Letters*, **2015**, 15, 6229-38	11.5	64
142	BoltzWann: A code for the evaluation of thermoelectric and electronic transport properties with a maximally-localized Wannier functions basis. *Computer Physics Communications*, **2014**, 185, 422-429	4.2	166
141	Piecewise linearity and spectroscopic properties from Koopmans-compliant functionals. *Topics in Current Chemistry*, **2014**, 347, 193-233		16
140	Thermal conductivity of graphene and graphite: collective excitations and mean free paths. *Nano Letters*, **2014**, 14, 6109-14	11.5	353
139	An Open-Source Multiscale Framework for the Simulation of Nanoscale Devices. *IEEE Transactions on Electron Devices*, **2014**, 61, 48-53	2.9	40
138	Phonon-limited resistivity of graphene by first-principles calculations: Electron-phonon interactions, strain-induced gauge field, and Boltzmann equation. *Physical Review B*, **2014**, 90,	3.3	76
137	Bridging density-functional and many-body perturbation theory: Orbital-density dependence in electronic-structure functionals. *Physical Review B*, **2014**, 89,	3.3	26
136	Engineering polar discontinuities in honeycomb lattices. *Nature Communications*, **2014**, 5, 5157	17.4	37
135	Electron-phonon interactions and the intrinsic electrical resistivity of graphene. *Nano Letters*, **2014**, 14, 1113-9	11.5	109
134	An updated version of BoltzWann: A code for the evaluation of thermoelectric and electronic transport properties with a maximally-localized Wannier functions basis. *Computer Physics Communications*, **2014**, 185, 2311-2312	4.2	8
133	Chemisorbed Molecules under Potential Bias: Detailed Insights from First-Principles Vibrational Spectroscopies. *Electrochimica Acta*, **2014**, 121, 210-214	6.7	21
132	Electrostatics of solvated systems in periodic boundary conditions. *Physical Review B*, **2014**, 90,	3.3	60

131	Spin-resolved optical conductivity of two-dimensional group-VIB transition-metal dichalcogenides. *Physical Review B*, **2014**, 90,	3.3	29
130	Koopmans-compliant functionals and their performance against reference molecular data. *Physical Review B*, **2014**, 90,	3.3	63
129	Static dielectric permittivity of ice from first principles. *Physical Review Letters*, **2014**, 113, 245501	7.4	7
128	An updated version of wannier90: A tool for obtaining maximally-localised Wannier functions. *Computer Physics Communications*, **2014**, 185, 2309-2310	4.2	949
127	First-Principles Determination of Phonon Lifetimes, Mean Free Paths, and Thermal Conductivities in Crystalline Materials: Pure Silicon and Germanium. *Topics in Applied Physics*, **2014**, 115-136	0.5	8
126	Covalently Functionalized Metallic Single-Walled Carbon Nanotubes Studied Using Electrostatic Force Microscopy and Dielectric Force Microscopy. *Journal of Physical Chemistry C*, **2013**, 117, 24570-24578	4.8	8
125	Defect ordering and defect□domain-wall interactions in PbTiO3: A first-principles study. *Physical Review B*, **2013**, 88,	3.3	75
124	Conductance Switching and Many-Valued Logic in Porphyrin Assemblies. *Journal of Physical Chemistry Letters*, **2013**, 4, 3039-3044	6.4	24
123	Donor and acceptor levels of organic photovoltaic compounds from first principles. *Physical Chemistry Chemical Physics*, **2013**, 15, 685-95	3.6	33
122	Self-assembled quantum dots in a nanowire system for quantum photonics. *Nature Materials*, **2013**, 12, 439-44	27	278
121	First-principles prediction of the equilibrium shape of nanoparticles under realistic electrochemical conditions. *Physical Review Letters*, **2013**, 110, 086104	7.4	50
120	Quantum states of muons in fluorides. *Physical Review B*, **2013**, 87,	3.3	37
119	First-principles quantum transport with electron-vibration interactions: A maximally localized Wannier functions approach. *Physical Review B*, **2013**, 87,	3.3	15
118	Surface composition tuning of Au-Pt bimetallic nanoparticles for enhanced carbon monoxide and methanol electro-oxidation. *Journal of the American Chemical Society*, **2013**, 135, 7985-91	16.4	240
117	A Natural Helical Crystal Lattice Model for Carbon Nanotubes. *Journal of Chemical Theory and Computation*, **2013**, 9, 1865-71	6.4	3
116	Thermodynamic stability of alkali-metal□inc double-cation borohydrides at low temperatures. *Physical Review B*, **2013**, 88,	3.3	27
115	Self-consistent continuum solvation (SCCS): the case of charged systems. *Journal of Chemical Physics*, **2013**, 139, 214110	3.9	73
114	Playing quantum hide-and-seek with the muon: localizing muon stopping sites. *Physica Scripta*, **2013**, 88, 068510	2.6	48

113	Diameter Effect on the Sidewall Functionalization of Single-Walled Carbon Nanotubes by Addition of Dichlorocarbene. *Advanced Functional Materials*, **2012**, 22, 5216-5223	15.6	12
112	Acoustic phonon lifetimes and thermal transport in free-standing and strained graphene. *Nano Letters*, **2012**, 12, 2673-8	11.5	154
111	Maximally localized Wannier functions: Theory and applications. *Reviews of Modern Physics*, **2012**, 84, 1419-1475	40.5	1475
110	The shear mode of multilayer graphene. *Nature Materials*, **2012**, 11, 294-300	27	482
109	Dominant phonon wave vectors and strain-induced splitting of the 2D Raman mode of graphene. *Physical Review B*, **2012**, 85,	3.3	31
108	Revised self-consistent continuum solvation in electronic-structure calculations. *Journal of Chemical Physics*, **2012**, 136, 064102	3.9	293
107	Electronic, vibrational, and transport properties of pnictogen-substituted ternary skutterudites. *Physical Review B*, **2012**, 85,	3.3	22
106	An integrated framework for multi-scale multi-physics numerical modelling of interface evolution in welding. *IOP Conference Series: Materials Science and Engineering*, **2012**, 33, 012029	0.4	4
105	Transport properties of room-temperature ionic liquids from classical molecular dynamics. *Journal of Chemical Physics*, **2012**, 137, 044508	3.9	32
104	Accurate potential energy surfaces with a DFT+U(R) approach. *Journal of Chemical Physics*, **2011**, 135, 194105	3.9	56
103	Improving the electrical conductivity of carbon nanotube networks: a first-principles study. *ACS Nano*, **2011**, 5, 9726-36	16.7	53
102	Berry phase and pseudospin winding number in bilayer graphene. *Physical Review B*, **2011**, 84,	3.3	64
101	Photoelectron properties of DNA and RNA bases from many-body perturbation theory. *Physical Review B*, **2011**, 84,	3.3	32
100	Switchable conductance in functionalized carbon nanotubes via reversible sidewall bond cleavage. *ACS Nano*, **2011**, 5, 4455-65	16.7	11
99	Accelerating GW calculations with optimal polarizability basis. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 527-536	1.3	14
98	Dominant phonon wavevectors of the 2D Raman mode of graphene. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 2635-2638	1.3	8
97	Carbene-functionalized single-walled carbon nanotubes and their electrical properties. *Small*, **2011**, 7, 1257-63	11	20
96	Role of disorder and anharmonicity in the thermal conductivity of silicon-germanium alloys: a first-principles study. *Physical Review Letters*, **2011**, 106, 045901	7.4	332

95	Transition-metal dioxides: a case for the intersite term in Hubbard-model functionals. *Journal of Chemical Physics*, **2011**, 134, 094103	3.9	43
94	Electrochemical Windows of Room-Temperature Ionic Liquids from Molecular Dynamics and Density Functional Theory Calculations. *Chemistry of Materials*, **2011**, 23, 2979-2986	9.6	271
93	High thermal conductivity in short-period superlattices. *Nano Letters*, **2011**, 11, 5135-41	11.5	75
92	Automated quantum conductance calculations using maximally-localised Wannier functions. *Computer Physics Communications*, **2011**, 182, 2174-2183	4.2	24
91	Accelerating GW Calculations with Optimal Polarizability Basis **2011**, 61-78		
90	Systematic study of first-row transition-metal diatomic molecules: a self-consistent DFT+U approach. *Journal of Chemical Physics*, **2010**, 133, 114103	3.9	73
89	Spatially extended Kondo state in magnetic molecules induced by interfacial charge transfer. *Physical Review Letters*, **2010**, 105, 106601	7.4	77
88	Local effects in the X-ray absorption spectrum of salt water. *Journal of Physical Chemistry B*, **2010**, 114, 9594-601	3.4	38
87	Effects of filling in CoSb3: Local structure, band gap, and phonons from first principles. *Physical Review B*, **2010**, 81,	3.3	60
86	Ultraviolet Photodetectors Based on Anodic TiO2 Nanotube Arrays. *Journal of Physical Chemistry C*, **2010**, 114, 10725-10729	3.8	206
85	Koopmans□condition for density-functional theory. *Physical Review B*, **2010**, 82,	3.3	176
84	Ab initio converse NMR approach for pseudopotentials. *Physical Review B*, **2010**, 81,	3.3	22
83	Ab Initio Electrochemical Properties of Electrode Surfaces **2010**, 415-431		14
82	Electronic Structure and Reactivity of Transition Metal Complexes **2010**, 433-455		3
81	Quantitative Description of Electron Transfer Reactions **2010**, 457-487		
80	Dynamics and thermodynamics of a novel phase of NaAlH4. *Physical Review Letters*, **2009**, 103, 185901	7.4	19
79	Electronic structure and transport properties of ternary skutterudite: CoX3/2Y3/2. *Materials Research Society Symposia Proceedings*, **2009**, 1166, 4		
78	Direct and Indirect Effects of Filling on Electronic Structure of Skutterudites. *Materials Research Society Symposia Proceedings*, **2009**, 1166, 7		1

77	NMR shifts for polycyclic aromatic hydrocarbons from first-principles. *International Journal of Quantum Chemistry*, **2009**, 109, 3336-3342	2.1	34
76	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. *Journal of Physics Condensed Matter*, **2009**, 21, 395502	1.8	13251
75	Linear and nonlinear susceptibilities from diffusion quantum Monte Carlo: application to periodic hydrogen chains. *Journal of Chemical Physics*, **2009**, 131, 094104	3.9	10
74	First-principles study of non-heme Fe(II) halogenase SyrB2 reactivity. *Journal of the American Chemical Society*, **2009**, 131, 14426-33	16.4	43
73	First-principles characterization of the structure and electronic structure of Ru and Rh-S chalcogenides. *Physical Review B*, **2009**, 80,	3.3	21
72	A converse approach to the calculation of NMR shielding tensors. *Journal of Chemical Physics*, **2009**, 131, 101101	3.9	49
71	Spin channels in functionalized graphene nanoribbons. *Nano Letters*, **2009**, 9, 3425-9	11.5	91
70	Surface energies, work functions, and surface relaxations of low-index metallic surfaces from first principles. *Physical Review B*, **2009**, 80,	3.3	340
69	Sensing mechanisms for carbon nanotube based NH3 gas detection. *Nano Letters*, **2009**, 9, 1626-30	11.5	191
68	Uniaxial strain in graphene by Raman spectroscopy: G peak splitting, Grüneisen parameters, and sample orientation. *Physical Review B*, **2009**, 79,	3.3	1422
67	Bulk aluminum at high pressure: A first-principles study. *Physical Review B*, **2008**, 77,	3.3	32
66	Unique carbon-nanotube field-effect transistors with asymmetric source and drain contacts. *Nano Letters*, **2008**, 8, 64-8	11.5	31
65	Global and local charge trapping in carbon nanotube field-effect transistors. *Nanotechnology*, **2008**, 19, 175203	3.4	7
64	The role of nanostructure in the wetting behavior of mixed-monolayer-protected metal nanoparticles. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 9886-91	11.5	98
63	Cycloadditions to Control Bond Breaking in Naphthalenes, Fullerenes, and Carbon Nanotubes: A First-Principles Study. *Journal of Physical Chemistry C*, **2008**, 112, 4480-4485	3.8	19
62	Electrostatics in periodic boundary conditions and real-space corrections. *Physical Review B*, **2008**, 77,	3.3	99
61	A self-consistent Hubbard U density-functional theory approach to the addition-elimination reactions of hydrocarbons on bare FeO+. *Journal of Chemical Physics*, **2008**, 129, 134314	3.9	61
60	Study of gaseous interactions in carbon nanotube field-effect transistors through selective Si(3)N(4) passivation. *Nanotechnology*, **2008**, 19, 465201	3.4	7

59	Lattice anharmonicity in low-dimensional carbon systems. *Physica Status Solidi (B): Basic Research*, **2008**, 245, 2149-2154	1.3	24
58	Theoretical study of the performance for short channel carbon nanotube transistors with asymmetric contacts. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2008**, 372, 6940-6943	2.3	3
57	Gate modulation in carbon nanotube field effect transistors-based NH3 gas sensors. *Sensors and Actuators B: Chemical*, **2008**, 132, 191-195	8.5	38
56	wannier90: A tool for obtaining maximally-localised Wannier functions. *Computer Physics Communications*, **2008**, 178, 685-699	4.2	2088
55	Simulation of heme using DFT + U: a step toward accurate spin-state energetics. *Journal of Physical Chemistry B*, **2007**, 111, 7384-91	3.4	122
54	SixC1□O2 alloys: A possible route to stabilize carbon-based silica-like solids?. *Solid State Communications*, **2007**, 144, 273-276	1.6	14
53	Phonon anharmonicities in graphite and graphene. *Physical Review Letters*, **2007**, 99, 176802	7.4	327
52	Car□arrinello molecular dynamics in the DFT+U formalism: Structure and energetics of solvated ferrous and ferric ions. *Journal of Electroanalytical Chemistry*, **2007**, 607, 107-112	4.1	16
51	In-plane structure and ordering at liquid sodium surfaces and interfaces from ab initio molecular dynamics. *Journal of Chemical Physics*, **2007**, 127, 134703	3.9	9
50	Exponential localization of Wannier functions in insulators. *Physical Review Letters*, **2007**, 98, 046402	7.4	235
49	Proton dynamics in superprotonic CsHSO4. *Physical Review B*, **2007**, 76,	3.3	67
48	Hydrogen bonding and coordination in normal and supercritical water from x-ray inelastic scattering. *Physical Review B*, **2007**, 76,	3.3	42
47	Vibrational recognition of adsorption sites for CO on platinum and platinum-ruthenium surfaces. *Journal of the American Chemical Society*, **2007**, 129, 11045-52	16.4	36
46	Spin and orbital magnetic response in metals: Susceptibility and NMR shifts. *Physical Review B*, **2007** , 76,	3.3	47
45	Stacking of oligo- and polythiophene cations in solution: surface tension and dielectric saturation. *Journal of Chemical Physics*, **2006**, 124, 194902	3.9	10
44	Dynamical structure, bonding, and thermodynamics of the superionic sublattice in alpha-AgI. *Physical Review Letters*, **2006**, 97, 166401	7.4	25
43	Ab initio studies of layering behavior of liquid sodium surfaces and interfaces. *Journal of Chemical Physics*, **2006**, 124, 174702	3.9	15
42	Realistic quantitative descriptions of electron transfer reactions: diabatic free-energy surfaces from first-principles molecular dynamics. *Physical Review Letters*, **2006**, 97, 028303	7.4	53

41	Realistic Modeling of Nanostructures Using Density Functional Theory. *MRS Bulletin*, **2006**, 31, 681-687	3.2	21
40	Cycloaddition functionalizations to preserve or control the conductance of carbon nanotubes. *Physical Review Letters*, **2006**, 97, 116801	7.4	108
39	Density functional theory in transition-metal chemistry: a self-consistent Hubbard U approach. *Physical Review Letters*, **2006**, 97, 103001	7.4	421
38	A unified electrostatic and cavitation model for first-principles molecular dynamics in solution. *Journal of Chemical Physics*, **2006**, 124, 74103	3.9	101
37	Effect of counterions on the interactions of charged oligothiophenes. *Journal of Physical Chemistry B*, **2006**, 110, 24822-6	3.4	12
36	Layering at liquid metal surfaces: Friedel oscillations and confinement effects. *Journal of Physics Condensed Matter*, **2006**, 18, L269-L275	1.8	9
35	Static dielectric properties of carbon nanotubes from first principles. *Physical Review Letters*, **2006**, 96, 166801	7.4	195
34	pi-Stacking in thiophene oligomers as the driving force for electroactive materials and devices. *Journal of the American Chemical Society*, **2005**, 127, 3207-12	16.4	69
33	Electronic-enthalpy functional for finite systems under pressure. *Physical Review Letters*, **2005**, 94, 145501	7.4	40
32	Band structure and quantum conductance of nanostructures from maximally localized Wannier functions: the case of functionalized carbon nanotubes. *Physical Review Letters*, **2005**, 95, 076804	7.4	152
31	First-principles determination of the structural, vibrational and thermodynamic properties of diamond, graphite, and derivatives. *Physical Review B*, **2005**, 71,	3.3	823
30	Dielectric response of periodic systems from quantum Monte Carlo calculations. *Physical Review Letters*, **2005**, 95, 207602	7.4	22
29	Static and dynamical properties of heavy water at ambient conditions from first-principles molecular dynamics. *Journal of Chemical Physics*, **2005**, 122, 204510	3.9	177
28	Phonon Dispersions of a Single-Wall (8,0) Carbon Nanotube: Effects of the Rotational Acoustic Sum Rule and of Surface Attachment. *Materials Research Society Symposia Proceedings*, **2004**, 858, 220		0
27	Stacking in Charged Thiophene Oligomers. *Journal of Physical Chemistry B*, **2004**, 108, 17791-17795	3.4	55
26	Mechanism of the Hydrogen/Platinum(111) Fuel Cell *Journal of Physical Chemistry B*, **2004**, 108, 19670-19680	3.4	9
25	Ab initiomolecular dynamics of metal surfaces. *Journal of Physics Condensed Matter*, **2004**, 16, S2575-S2586	1.8	17
24	Ab initio transport properties of nanostructures from maximally localized Wannier functions. *Physical Review B*, **2004**, 69,	3.3	220

23	Photoinduced oxidation of carbon nanotubes. *Journal of Physics Condensed Matter*, **2003**, 15, 5915-5921	1.8	87
22	The electroreduction of hydrogen on platinum(111) in acidic media. *Journal of Electroanalytical Chemistry*, **2002**, 537, 7-19	4.1	16
21	Maximally localized Wannier functions in antiferromagnetic MnO within the FLAPW formalism. *Physical Review B*, **2002**, 65,	3.3	29
20	A classical and ab initio study of the interaction of the myosin triphosphate binding domain with ATP. *Biophysical Journal*, **2002**, 82, 660-75	2.9	33
19	Maximally localized Wannier functions for entangled energy bands. *Physical Review B*, **2001**, 65,	3.3	1174
18	Wannier functions characterization of floating bonds in a-Si. *Computational Materials Science*, **2001**, 20, 337-342	3.2	9
17	Ab initio determination of the dielectric response of GaAs, AlAs, C, and SrO in the weighted-density approximation. *Journal of Physics and Chemistry of Solids*, **2000**, 61, 321-325	3.9	8
16	Insight into gallium behavior in aluminum grain boundaries from calculation on Σ11 (113) boundary. *Acta Materialia*, **2000**, 48, 3623-3632	8.4	44
15	Dielectric response of oxides in the weighted density approximation. *Physical Review B*, **2000**, 62, 12724-12729	3.3	55
14	Wannier-function description of the electronic polarization and infrared absorption of high-pressure hydrogen. *Physical Review B*, **2000**, 62, 15505-15520	3.3	17
13	Thermal Contraction and Disordering of the Al(110) Surface. *Physical Review Letters*, **1999**, 82, 3296-3299	7.4	700
12	Maximally-localized Wannier functions for disordered systems: Application to amorphous silicon. *Solid State Communications*, **1998**, 107, 7-11	1.6	320
11	First principles calculation of the energy and structure of two solid surface phases on Ir{100}. *Surface Science*, **1998**, 418, 529-535	1.8	34
10	Maximally-localized Wannier functions in perovskites: Cubic BaTiO3 **1998**,		6
9	Sliding Mechanisms in Aluminum Grain Boundaries. *Physical Review Letters*, **1997**, 79, 869-872	7.4	65
8	Maximally localized generalized Wannier functions for composite energy bands. *Physical Review B*, **1997**, 56, 12847-12865	3.3	2886
7	Ensemble Density-Functional Theory for Ab Initio Molecular Dynamics of Metals and Finite-Temperature Insulators. *Physical Review Letters*, **1997**, 79, 1337-1340	7.4	277
6	Ab Initio Investigation of Grain Boundary Sliding. *Materials Research Society Symposia Proceedings*, **1995**, 408, 283		

5	Structure and phase stability of GaxIn1-xP solid solutions from computational alchemy. *Physical Review Letters*, **1994**, 72, 4001-4004	7.4	56
4	A Mori-Tanaka Theory for Textured Short-Fiber Composites: Application. *Journal of Energy Resources Technology, Transactions of the ASME*, **1992**, 114, 101-104	2.6	8
3	Textural and Micromorphological Effects on the Overall Elastic Response of Macroscopically Anisotropic Composites. *Journal of Applied Mechanics, Transactions ASME*, **1992**, 59, 269-275	2.7	45
2	Data Management Plans: the Importance of Data Management in the BIG-MAP Project□**. *Batteries and Supercaps*,	5.6	6
1	Virtual Computational Chemistry Teaching Laboratories□Hands-On at a Distance. *Journal of Chemical Education*,	2.4	5