Jeffrey B Neaton

List of Publications by Citations

245 papers	25,038 citations	78 h-index	155 g-index
261 ext. papers	28,115 ext. citations	9.1 avg, IF	7.08 L-index

#	Paper	IF	Citations
245	Epitaxial BiFeO3 multiferroic thin film heterostructures. *Science*, **2003**, 299, 1719-22	33.3	4944
244	First-principles study of metal adatom adsorption on graphene. *Physical Review B*, **2008**, 77,	3.3	1104
243	First-principles study of spontaneous polarization in multiferroic BiFeO3. *Physical Review B*, **2005**, 71,	3.3	1058
242	Cooperative insertion of CO2 in diamine-appended metal-organic frameworks. *Nature*, **2015**, 519, 303-8	50.4	807
241	Renormalization of molecular electronic levels at metal-molecule interfaces. *Physical Review Letters*, **2006**, 97, 216405	7.4	693
240	Synthesis, characterization, and theory of [9]-, [12]-, and [18]cycloparaphenylene: carbon nanohoop structures. *Journal of the American Chemical Society*, **2008**, 130, 17646-7	16.4	650
239	Mechanically controlled binary conductance switching of a single-molecule junction. *Nature Nanotechnology*, **2009**, 4, 230-4	28.7	515
238	Amine-gold linked single-molecule circuits: experiment and theory. *Nano Letters*, **2007**, 7, 3477-82	11.5	403
237	Elastic properties of chemical-vapor-deposited monolayer MoS2, WS2, and their bilayer heterostructures. *Nano Letters*, **2014**, 14, 5097-103	11.5	384
236	Pairing in dense lithium. *Nature*, **1999**, 400, 141-144	50.4	328
235	First-principles study of the structure and lattice dielectric response of CaCu3Ti4O12. *Physical Review B*, **2002**, 65,	3.3	301
234	Theory of polarization enhancement in epitaxial BaTiO3/SrTiO3 superlattices. *Applied Physics Letters*, **2003**, 82, 1586-1588	3.4	296
233	Extrinsic models for the dielectric response of CaCu3Ti4O12. *Journal of Applied Physics*, **2003**, 94, 3299-3306	2.5	295
232	Single-molecule diodes with high rectification ratios through environmental control. *Nature Nanotechnology*, **2015**, 10, 522-7	28.7	278
231	Comprehensive study of carbon dioxide adsorption in the metal-organic frameworks M2(dobdc) (M = Mg, Mn, Fe, Co, Ni, Cu, Zn). *Chemical Science*, **2014**, 5, 4569-4581	9.4	267
230	Theory and computation of hot carriers generated by surface plasmon polaritons in noble metals. *Nature Communications*, **2015**, 6, 7044	17.4	238
229	Simultaneous determination of conductance and thermopower of single molecule junctions. *Nano Letters*, **2012**, 12, 354-8	11.5	217

228	GW100: Benchmarking G0W0 for Molecular Systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 5665-87	6.4	207
227	Defect-Induced Band-Edge Reconstruction of a Bismuth-Halide Double Perovskite for Visible-Light Absorption. *Journal of the American Chemical Society*, **2017**, 139, 5015-5018	16.4	206
226	Quasiparticle spectra from a nonempirical optimally tuned range-separated hybrid density functional. *Physical Review Letters*, **2012**, 109, 226405	7.4	203
225	Ab initio study of the phase diagram of epitaxial BaTiO3. *Physical Review B*, **2004**, 69,	3.3	201
224	Small-Molecule Adsorption in Open-Site Metal□Organic Frameworks: A Systematic Density Functional Theory Study for Rational Design. *Chemistry of Materials*, **2015**, 27, 668-678	9.6	198
223	Layered Halide Double Perovskites: Dimensional Reduction of CsAgBiBr. *Journal of the American Chemical Society*, **2018**, 140, 5235-5240	16.4	197
222	Gap renormalization of molecular crystals from density-functional theory. *Physical Review B*, **2013**, 88,	3.3	197
221	Electron delocalization and charge mobility as a function of reduction in a metal-organic framework. *Nature Materials*, **2018**, 17, 625-632	27	182
220	The mechanism of carbon dioxide adsorption in an alkylamine-functionalized metal-organic framework. *Journal of the American Chemical Society*, **2013**, 135, 7402-5	16.4	175
219	Solid-state optical absorption from optimally tuned time-dependent range-separated hybrid density functional theory. *Physical Review B*, **2015**, 92,	3.3	171
218	ab initio study of hot carriers in the first picosecond after sunlight absorption in silicon. *Physical Review Letters*, **2014**, 112, 257402	7.4	166
217	Tunability of the dielectric response of epitaxially strained SrTiO3 from first principles. *Physical Review B*, **2005**, 71,	3.3	162
216	Reversible CO binding enables tunable CO/H□and CO/N□separations in metal-organic frameworks with exposed divalent metal cations. *Journal of the American Chemical Society*, **2014**, 136, 10752-61	16.4	160
215	Conductance and geometry of pyridine-linked single-molecule junctions. *Journal of the American Chemical Society*, **2010**, 132, 6817-21	16.4	160
214	Quasiparticle and optical spectroscopy of the organic semiconductors pentacene and PTCDA from first principles. *Physical Review B*, **2012**, 85,	3.3	158
213	Charge density wave order in 1D mirror twin boundaries of single-layer MoSe2. *Nature Physics*, **2016**, 12, 751-756	16.2	156
212	Tuning rectification in single-molecular diodes. *Nano Letters*, **2013**, 13, 6233-7	11.5	152
211	Negative differential resistance in carbon atomic wire-carbon nanotube junctions. *Nano Letters*, **2008**, 8, 2900-5	11.5	152

210	Structural, electronic, and magnetic properties of SrRuO3 under epitaxial strain. *Physical Review B*, **2006**, 74,	3.3	147
209	Atomate: A high-level interface to generate, execute, and analyze computational materials science workflows. *Computational Materials Science*, **2017**, 139, 140-152	3.2	142
208	Low-Energy Charge-Transfer Excitons in Organic Solids from First-Principles: The Case of Pentacene. *Journal of Physical Chemistry Letters*, **2013**, 4, 2197-2201	6.4	136
207	Enrichment of molecular antenna triplets amplifies upconverting nanoparticle emission. *Nature Photonics*, **2018**, 12, 402-407	33.9	135
206	Length dependence of conductance in aromatic single-molecule junctions. *Nano Letters*, **2009**, 9, 3949-53	11.5	135
205	Design of a metal-organic framework with enhanced back bonding for separation of N□and CH□ *Journal of the American Chemical Society*, **2014**, 136, 698-704	16.4	134
204	On the constitution of sodium at higher densities. *Physical Review Letters*, **2001**, 86, 2830-3	7.4	131
203	Inversion symmetry and bulk Rashba effect in methylammonium lead iodide perovskite single crystals. *Nature Communications*, **2018**, 9, 1829	17.4	123
202	First-principles study of symmetry lowering and polarization in BaTiO3□SrTiO3 superlattices with in-plane expansion. *Physical Review B*, **2005**, 71,	3.3	121
201	Identifying substitutional oxygen as a prolific point defect in monolayer transition metal dichalcogenides. *Nature Communications*, **2019**, 10, 3382	17.4	117
200	Charge separation via strain in silicon nanowires. *Nano Letters*, **2009**, 9, 2418-22	11.5	116
199	Band gap and edge engineering via ferroic distortion and anisotropic strain: the case of SrTiO(3). *Physical Review Letters*, **2011**, 107, 146804	7.4	115
198	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
197	Non-chemisorbed gold-sulfur binding prevails in self-assembled monolayers. *Nature Chemistry*, **2019**, 11, 351-358	17.6	113
196	A systematic benchmark of the ab initio Bethe-Salpeter equation approach for low-lying optical excitations of small organic molecules. *Journal of Chemical Physics*, **2015**, 142, 244101	3.9	113
195	Understanding Trends in CO2 Adsorption in Metal-Organic Frameworks with Open-Metal Sites. *Journal of Physical Chemistry Letters*, **2014**, 5, 861-5	6.4	113
194	Solar fuels photoanode materials discovery by integrating high-throughput theory and experiment. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 3040-3043	11.5	111
193	Cooperative carbon capture and steam regeneration with tetraamine-appended metal-organic frameworks. *Science*, **2020**, 369, 392-396	33.3	111

192	Outer-valence Electron Spectra of Prototypical Aromatic Heterocycles from an Optimally Tuned Range-Separated Hybrid Functional. *Journal of Chemical Theory and Computation*, **2014**, 10, 1934-1952	6.4	109
191	Chemical Raman enhancement of organic adsorbates on metal surfaces. *Physical Review Letters*, **2011**, 106, 083003	7.4	109
190	Large Bulk Photovoltaic Effect and Spontaneous Polarization of Single-Layer Monochalcogenides. *Physical Review Letters*, **2017**, 119, 067402	7.4	104
189	Electronic properties of the Si/SiO2 interface from first principles. *Physical Review Letters*, **2000**, 85, 1298-301	7.4	104
188	Tuning semiconductor band edge energies for solar photocatalysis via surface ligand passivation. *Nano Letters*, **2012**, 12, 383-8	11.5	103
187	molgw 1: Many-body perturbation theory software for atoms, molecules, and clusters. *Computer Physics Communications*, **2016**, 208, 149-161	4.2	97
186	Force-Field Development from Electronic Structure Calculations with Periodic Boundary Conditions: Applications to Gaseous Adsorption and Transport in Metal-Organic Frameworks. *Journal of Chemical Theory and Computation*, **2014**, 10, 1477-88	6.4	97
185	Strain-induced band gap modification in coherent core/shell nanostructures. *Nano Letters*, **2010**, 10, 3156-62	11.5	97
184	Electronic energy levels of weakly coupled nanostructures: C60-metal interfaces. *Physical Review Letters*, **2008**, 101, 026804	7.4	95
183	Determination of energy level alignment and coupling strength in 4,4′-bipyridine single-molecule junctions. *Nano Letters*, **2014**, 14, 794-8	11.5	93
182	Ab initio study of hot electrons in GaAs. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 5291-6	11.5	92
181	Relating energy level alignment and amine-linked single molecule junction conductance. *Nano Letters*, **2010**, 10, 2470-4	11.5	92
180	Environmental control of single-molecule junction transport. *Nano Letters*, **2011**, 11, 1988-92	11.5	91
179	Detection of sub-MeV dark matter with three-dimensional Dirac materials. *Physical Review D*, **2018**, 97,	4.9	90
178	Excited-state vibrational dynamics toward the polaron in methylammonium lead iodide perovskite. *Nature Communications*, **2018**, 9, 2525	17.4	90
177	Small-Band-Gap Halide Double Perovskites. *Angewandte Chemie - International Edition*, **2018**, 57, 12765-12770	12.1	89
176	Reliable energy level alignment at physisorbed molecule-metal interfaces from density functional theory. *Nano Letters*, **2015**, 15, 2448-55	11.5	88
175	CO2 capture by metal-organic frameworks with van der Waals density functionals. *Journal of Physical Chemistry A*, **2012**, 116, 4957-64	2.8	86

174	Lattice dielectric response of CdCu3Ti4O12 and CaCu3Ti4O12 from first principles. *Physical Review B*, **2003**, 67,	3.3	86
173	Molecular adsorption on metal surfaces with van der Waals density functionals. *Physical Review B*, **2012**, 85,	3.3	85
172	Tunable charge transport in single-molecule junctions via electrolytic gating. *Nano Letters*, **2014**, 14, 1400-4	11.5	84
171	Ligand-assisted enhancement of CO2 capture in metal-organic frameworks. *Journal of the American Chemical Society*, **2012**, 134, 6714-9	16.4	82
170	Manipulating magnetic properties of SrRuO3 and CaRuO3 with epitaxial and uniaxial strains. *Physical Review B*, **2008**, 77,	3.3	81
169	Thermopower of amine-gold-linked aromatic molecular junctions from first principles. *ACS Nano*, **2011**, 5, 551-7	16.7	79
168	Structural evidence for enhanced polarization in a commensurate short-period BaTiO3–SrTiO3 superlattice. *Applied Physics Letters*, **2006**, 89, 092905	3.4	78
167	First-principles study of adhesion at Cu/SiO2 interfaces. *Physical Review B*, **2003**, 68,	3.3	76
166	Charge transport and rectification in molecular junctions formed with carbon-based electrodes. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 10928-32	11.5	74
165	Electric Field- and Strain-Induced Rashba Effect in Hybrid Halide Perovskites. *Journal of Physical Chemistry Letters*, **2016**, 7, 3683-9	6.4	74
164	Structural and excited-state properties of oligoacene crystals from first principles. *Physical Review B*, **2016**, 93,	3.3	73
163	Formation of the layered conductive magnet CrCl(pyrazine) through redox-active coordination chemistry. *Nature Chemistry*, **2018**, 10, 1056-1061	17.6	73
162	Force Field Development from Periodic Density Functional Theory Calculations for Gas Separation Applications Using Metal–Organic Frameworks. *Journal of Physical Chemistry C*, **2016**, 120, 12590-12604	3.8	71
161	Control of single-molecule junction conductance of porphyrins via a transition-metal center. *Nano Letters*, **2014**, 14, 5365-70	11.5	70
160	High Throughput Discovery of Solar Fuels Photoanodes in the CuO–V2O5 System. *Advanced Energy Materials*, **2015**, 5, 1500968	21.8	70
159	Inverse rectification in donor-acceptor molecular heterojunctions. *ACS Nano*, **2011**, 5, 9256-63	16.7	70
158	Electronic energy level alignment at metal-molecule interfaces with a GW approach. *Physical Review B*, **2011**, 84,	3.3	69
157	Defect-Induced Modification of Low-Lying Excitons and Valley Selectivity in Monolayer Transition Metal Dichalcogenides. *Physical Review Letters*, **2018**, 121, 167402	7.4	69

156	Electronic level alignment at a metal-molecule interface from a short-range hybrid functional. *Journal of Chemical Physics*, **2011**, 135, 164706	3.9	65
155	Relating the Physical Structure and Optoelectronic Function of Crystalline TIPS-Pentacene. *Advanced Functional Materials*, **2015**, 25, 2038-2046	15.6	64
154	Quantum confinement and electronic properties of tapered silicon nanowires. *Physical Review Letters*, **2008**, 100, 246804	7.4	64
153	Excited-State Properties of Molecular Solids from First Principles. *Annual Review of Physical Chemistry*, **2016**, 67, 587-616	15.7	64
152	A reversible single-molecule switch based on activated antiaromaticity. *Science Advances*, **2017**, 3, eaao2615	14.3	63
151	Beyond Energies: Geometries of Nonbonded Molecular Complexes as Metrics for Assessing Electronic Structure Approaches. *Journal of Chemical Theory and Computation*, **2015**, 11, 1481-92	6.4	63
150	An assessment of low-lying excitation energies and triplet instabilities of organic molecules with an ab initio Bethe-Salpeter equation approach and the Tamm-Dancoff approximation. *Journal of Chemical Physics*, **2017**, 146, 194108	3.9	62
149	Quantitative current-voltage characteristics in molecular junctions from first principles. *Nano Letters*, **2012**, 12, 6250-4	11.5	62
148	Computational design of low-band-gap double perovskites. *Physical Review B*, **2012**, 86,	3.3	62
147	Epitaxial growth of multiferroic YMnO3 on GaN. *Applied Physics Letters*, **2005**, 87, 171915	3.4	61
146	Elucidating CO Chemisorption in Diamine-Appended Metal-Organic Frameworks. *Journal of the American Chemical Society*, **2018**, 140, 18016-18031	16.4	61
145	Evaluating the GW Approximation with CCSD(T) for Charged Excitations Across the Oligoacenes. *Journal of Chemical Theory and Computation*, **2016**, 12, 2834-42	6.4	60
144	Long-Lived Correlated Triplet Pairs in a π-Stacked Crystalline Pentacene Derivative. *Journal of the American Chemical Society*, **2018**, 140, 2326-2335	16.4	57
143	Low-energy linear structures in dense oxygen: implications for the epsilon phase. *Physical Review Letters*, **2002**, 88, 205503	7.4	56
142	Water Enables Efficient CO Capture from Natural Gas Flue Emissions in an Oxidation-Resistant Diamine-Appended Metal-Organic Framework. *Journal of the American Chemical Society*, **2019**, 141, 13171-13186	16.4	55
141	Voltage tuning of vibrational mode energies in single-molecule junctions. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 1282-7	11.5	55
140	Low-lying electronic excited states of pentacene oligomers: a comparative electronic structure study in the context of singlet fission. *Journal of Chemical Theory and Computation*, **2015**, 11, 147-56	6.4	55
139	Mechanical and charge transport properties of alkanethiol self-assembled monolayers on a au(111) surface: the role of molecular tilt. *Langmuir*, **2008**, 24, 2219-23	4	55

138	Electronically Transparent Au-N Bonds for Molecular Junctions. *Journal of the American Chemical Society*, **2017**, 139, 14845-14848	16.4	52
137	Mn2V2O7: An Earth Abundant Light Absorber for Solar Water Splitting. *Advanced Energy Materials*, **2015**, 5, 1401840	21.8	51
136	Negative differential resistance in transport through organic molecules on silicon. *Physical Review Letters*, **2007**, 98, 066807	7.4	50
135	Energy level alignment at molecule-metal interfaces from an optimally tuned range-separated hybrid functional. *Journal of Chemical Physics*, **2017**, 146, 092326	3.9	49
134	Assessing DFT-D3 Damping Functions Across Widely Used Density Functionals: Can We Do Better?. *Journal of Chemical Theory and Computation*, **2017**, 13, 2043-2052	6.4	48
133	Controlling the Thermoelectric Properties of Thiophene-Derived Single-Molecule Junctions. *Chemistry of Materials*, **2014**, 26, 7229-7235	9.6	48
132	Quantitative molecular orbital energies within a G0W0 approximation. *European Physical Journal B*, **2012**, 85, 1	1.2	48
131	Using Molecular Design to Control the Performance of Hydrogen-Producing Polymer-Brush-Modified Photocathodes. *Journal of Physical Chemistry Letters*, **2014**, 5, 3222-6	6.4	47
130	Probing adsorption interactions in metal-organic frameworks using X-ray spectroscopy. *Journal of the American Chemical Society*, **2013**, 135, 18183-90	16.4	47
129	First-principles Hubbard U approach for small molecule binding in metal-organic frameworks. *Journal of Chemical Physics*, **2016**, 144, 174104	3.9	47
128	Effect of reduced dimensionality on the optical band gap of SrTiO3. *Applied Physics Letters*, **2013**, 102, 122901	3.4	45
127	Stability and self-passivation of copper vanadate photoanodes under chemical, electrochemical, and photoelectrochemical operation. *Physical Chemistry Chemical Physics*, **2016**, 18, 9349-52	3.6	45
126	Mapping the Transmission Functions of Single-Molecule Junctions. *Nano Letters*, **2016**, 16, 3949-54	11.5	43
125	Simultaneous Determination of Structures, Vibrations, and Frontier Orbital Energies from a Self-Consistent Range-Separated Hybrid Functional. *Journal of Physical Chemistry Letters*, **2014**, 5, 2734-41	6.4	43
124	Density functional theory based calculation of small-polaron mobility in hematite. *Physical Review B* , **2014**, 89,	3.3	43
123	Relating Trends in First-Principles Electronic Structure and Open-Circuit Voltage in Organic Photovoltaics. *Journal of Physical Chemistry Letters*, **2011**, 2, 2531-2537	6.4	43
122	Solar fuel photoanodes prepared by inkjet printing of copper vanadates. *Journal of Materials Chemistry A*, **2016**, 4, 7483-7494	13	43
121	CO induced phase transitions in diamine-appended metal-organic frameworks. *Chemical Science*, **2015**, 6, 5177-5185	9.4	42

120	Origins of Singlet Fission in Solid Pentacene from an ab initio Green's Function Approach. *Physical Review Letters*, **2017**, 119, 267401	7.4	42
119	Ab initio electronic relaxation times and transport in noble metals. *Physical Review B*, **2016**, 94,	3.3	40
118	Carrier Diffusion Lengths Exceeding 1 μm in Despite Trap-Limited Transport in Halide Double Perovskites. *ACS Energy Letters*, **2020**, 5, 1337-1345	20.1	39
117	Formation of Y2O3 nanoclusters in nanostructured ferritic alloys during isothermal and anisothermal heat treatment: A kinetic Monte Carlo study. *Physical Review B*, **2009**, 80,	3.3	38
116	Dirac metal to topological metal transition at a structural phase change in Au2Pb and prediction of Z2 topology for the superconductor. *Physical Review B*, **2015**, 91,	3.3	37
115	Transferable pair potentials for CdS and ZnS crystals. *Journal of Chemical Physics*, **2012**, 136, 234111	3.9	37
114	Tuning the bandgap of CsAgBiBr through dilute tin alloying. *Chemical Science*, **2019**, 10, 10620-10628	9.4	37
113	Nonperturbative visualization of nanoscale plasmonic field distributions via photon localization microscopy. *Physical Review Letters*, **2011**, 106, 037402	7.4	36
112	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
111	Probing the mechanism of CO2 capture in diamine-appended metal-organic frameworks using measured and simulated X-ray spectroscopy. *Physical Chemistry Chemical Physics*, **2015**, 17, 21448-57	3.6	35
110	Quantitative Prediction of Optical Absorption in Molecular Solids from an Optimally Tuned Screened Range-Separated Hybrid Functional. *Journal of Chemical Theory and Computation*, **2018**, 14, 2919-2929	6.4	34
109	Observation of a two-dimensional Fermi surface and Dirac dispersion in YbMnSb2. *Physical Review B*, **2018**, 97,	3.3	33
108	Ab initio phonon dispersion in crystalline naphthalene using van der Waals density functionals. *Physical Review B*, **2016**, 93,	3.3	33
107	Structure and electronic properties of cerium orthophosphate: Theory and experiment. *Physical Review B*, **2011**, 83,	3.3	33
106	Performance of van der Waals Corrected Functionals for Guest Adsorption in the M(dobdc) Metal-Organic Frameworks. *Journal of Physical Chemistry A*, **2017**, 121, 4139-4151	2.8	32
105	Parameter-free driven Liouville-von Neumann approach for time-dependent electronic transport simulations in open quantum systems. *Journal of Chemical Physics*, **2017**, 146, 092331	3.9	32
104	Topological materials discovery using electron filling constraints. *Nature Physics*, **2018**, 14, 55-61	16.2	32
103	Interplay of Bias-Driven Charging and the Vibrational Stark Effect in Molecular Junctions. *Nano Letters*, **2016**, 16, 1104-9	11.5	32

102	Pairing, bonding, and the role of nonlocality in a dense lithium monolayer. *Physical Review B*, **2000**, 62, 8494-8499	3.3	32
101	Adsorption-Induced Solvent-Based Electrostatic Gating of Charge Transport through Molecular Junctions. *Nano Letters*, **2015**, 15, 4498-503	11.5	30
100	Understanding Small-Molecule Interactions in Metal-Organic Frameworks: Coupling Experiment with Theory. *Advanced Materials*, **2015**, 27, 5785-96	24	30
99	Cooperative Carbon Dioxide Adsorption in Alcoholamine- and Alkoxyalkylamine-Functionalized Metal-Organic Frameworks. *Angewandte Chemie - International Edition*, **2020**, 59, 19468-19477	16.4	30
98	Push it to the limit: Characterizing the convergence of common sequences of basis sets for intermolecular interactions as described by density functional theory. *Journal of Chemical Physics*, **2016**, 144, 194306	3.9	29
97	Assessment of two hybrid van der Waals density functionals for covalent and non-covalent binding of molecules. *Journal of Chemical Physics*, **2017**, 146, 234106	3.9	28
96	Enhancement of CO binding and mechanical properties upon diamine functionalization of M(dobpdc) metal-organic frameworks. *Chemical Science*, **2018**, 9, 5197-5206	9.4	28
95	Theory of Covalent Adsorbate Frontier Orbital Energies on Functionalized Light-Absorbing Semiconductor Surfaces. *Journal of Physical Chemistry Letters*, **2013**, 4, 1701-6	6.4	27
94	Discovery of Manganese-Based Solar Fuel Photoanodes via Integration of Electronic Structure Calculations, Pourbaix Stability Modeling, and High-Throughput Experiments. *ACS Energy Letters*, **2017**, 2, 2307-2312	20.1	25
93	Molecular-scale quantum dots from carbon nanotube heterojunctions. *Nano Letters*, **2009**, 9, 1544-8	11.5	25
92	Reducing Coercive-Field Scaling in Ferroelectric Thin Films via Orientation Control. *ACS Nano*, **2018**, 12, 4736-4743	16.7	24
91	Nonlinear variations in the electronic structure of II-VI and III-V wurtzite semiconductors with biaxial strain. *Applied Physics Letters*, **2011**, 98, 152108	3.4	24
90	Low-lying excited states in crystalline perylene. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 284-289	11.5	23
89	Harnessing Chemical Raman Enhancement for Understanding Organic Adsorbate Binding on Metal Surfaces. *Journal of Physical Chemistry Letters*, **2012**, 3, 1357-62	6.4	23
88	Probing Charge Transport through Peptide Bonds. *Journal of Physical Chemistry Letters*, **2018**, 9, 763-767	6.4	22
87	Mechanism for bias-assisted indium mass transport on carbon nanotube surfaces. *Physical Review B*, **2005**, 72,	3.3	22
86	Effects of self-consistency and plasmon-pole models on GW calculations for closed-shell molecules. *Physical Review B*, **2014**, 90,	3.3	21
85	Efficient Determination of Accurate Force Fields for Porous Materials Using ab Initio Total Energy Calculations. *Journal of Physical Chemistry C*, **2014**, 118, 2693-2701	3.8	21

84	Effective empirical corrections for basis set superposition error in the def2-SVPD basis: gCP and DFT-C. *Journal of Chemical Physics*, **2017**, 146, 234105	3.9	21
83	Successes and Opportunities for Discovery of Metal Oxide Photoanodes for Solar Fuels Generators. *ACS Energy Letters*, **2020**, 5, 1413-1421	20.1	19
82	First-principles studies of the dynamics of [2]rotaxane molecular switches. *Nano Letters*, **2009**, 9, 3225-9	11.5	19
81	An automatically curated first-principles database of ferroelectrics. *Scientific Data*, **2020**, 7, 72	8.2	18
80	Assessing electronic structure approaches for gas-ligand interactions in metal-organic frameworks: the CO2-benzene complex. *Journal of Chemical Physics*, **2014**, 140, 104707	3.9	18
79	Zigzag inversion domain boundaries in indium zinc oxide-based nanowires: structure and formation. *ACS Nano*, **2013**, 7, 10747-51	16.7	18
78	Ferromagnetic instabilities in atomically thin lithium and sodium wires. *International Journal of Quantum Chemistry*, **2003**, 91, 239-244	2.1	18
77	Towards predictive band gaps for halide perovskites: Lessons from one-shot and eigenvalue self-consistent GW. *Physical Review Materials*, **2019**, 3,	3.2	18
76	Real-space pseudopotential calculations of spin-dependent electron transport in magnetic molecular junctions. *Physical Review B*, **2007**, 76,	3.3	17
75	Origins of the Pressure-Induced Phase Transition and Metallization in the Halide Perovskite (CH3NH3)PbI3. *ACS Energy Letters*, **2020**, 5, 2174-2181	20.1	17
74	Accelerating GW-Based Energy Level Alignment Calculations for Molecule-Metal Interfaces Using a Substrate Screening Approach. *Journal of Chemical Theory and Computation*, **2019**, 15, 4218-4227	6.4	16
73	Ligand coupling symmetry correlates with thermopower enhancement in small-molecule/nanocrystal hybrid materials. *ACS Nano*, **2014**, 8, 10528-36	16.7	16
72	Voltage Dependence of Molecule–Electrode Coupling in Biased Molecular Junctions. *Journal of Physical Chemistry C*, **2017**, 121, 21136-21144	3.8	16
71	Flat branches and pressure amorphization. *Journal of Non-Crystalline Solids*, **2002**, 307-310, 602-612	3.9	16
70	A direct look at halogen bonds. *Science*, **2017**, 358, 167-168	33.3	15
69	Thermodynamic signature of Dirac electrons across a possible topological transition in ZrTe5. *Physical Review B*, **2018**, 97,	3.3	15
68	Phosphonic Acid Adsorbates Tune the Surface Potential of TiO2 in Gas and Liquid Environments. *Journal of Physical Chemistry Letters*, **2014**, 5, 2450-4	6.4	15
67	Ytterbium-driven strong enhancement of electron-phonon coupling in graphene. *Physical Review B*, **2014**, 90,	3.3	15

66	Reproducibility in G0W0 calculations for solids. *Computer Physics Communications*, **2020**, 255, 107242	4.2	14
65	Bi-Containing n-FeWO4 Thin Films Provide the Largest Photovoltage and Highest Stability for a Sub-2 eV Band Gap Photoanode. *ACS Energy Letters*, **2018**, 3, 2769-2774	20.1	14
64	Cooperative Gas Adsorption without a Phase Transition in Metal-Organic Frameworks. *Physical Review Letters*, **2018**, 121, 015701	7.4	13
63	Communication: energy-dependent resonance broadening in symmetric and asymmetric molecular junctions from an ab initio non-equilibrium Green@ function approach. *Journal of Chemical Physics*, **2014**, 141, 131104	3.9	13
62	Expanded Analogs of Three-Dimensional Lead-Halide Hybrid Perovskites. *Angewandte Chemie - International Edition*, **2020**, 59, 19087-19094	16.4	12
61	Small-Band-Gap Halide Double Perovskites. *Angewandte Chemie*, **2018**, 130, 12947-12952	3.6	12
60	First-principles study of electronic structure and photocatalytic properties of MnNiO3 as an alkaline oxygen-evolution photocatalyst. *Chemical Communications*, **2015**, 51, 2867-70	5.8	12
59	Directed assembly of layered perovskite heterostructures as single crystals. *Nature*, **2021**, 597, 355-359	50.4	12
58	Single-molecule junctions: thermoelectricity at the gate. *Nature Nanotechnology*, **2014**, 9, 876-7	28.7	11
57	Numerical integration for ab initio many-electron self energy calculations within the GW approximation. *Journal of Computational Physics*, **2015**, 286, 1-13	4.1	11
56	Competing thermodynamic and dynamic factors select molecular assemblies on a gold surface. *Physical Review Letters*, **2013**, 111, 265701	7.4	11
55	First-principles studies of the electronic structure of cyclopentene on Si(001): density functional theory and GW calculations. *Physica Status Solidi (B): Basic Research*, **2006**, 243, 2048-2053	1.3	11
54	Enhanced polarization in strained BaTiO3 from first principles. *Materials Research Society Symposia Proceedings*, **2002**, 718, 1		11
53	High Compression-Induced Conductivity in a Layered Cu-Br Perovskite. *Angewandte Chemie - International Edition*, **2020**, 59, 4017-4022	16.4	11
52	Chemically Localized Resonant Excitons in Silver-Pnictogen Halide Double Perovskites. *Journal of Physical Chemistry Letters*, **2021**, 12, 2057-2063	6.4	11
51	Contact dependence of the conductance of H2 molecular junctions from first principles. *Physical Review B*, **2008**, 77,	3.3	10
50	First-principles description of phonons in Ni50Pt50 disordered alloys: The role of relaxation. *Physical Review B*, **2004**, 70,	3.3	10
49	Fermi-crossing Type-II Dirac fermions and topological surface states in NiTe. *Scientific Reports*, **2020** , 10, 12957	4.9	10

48	Room-temperature skyrmion lattice in a layered magnet (FeCo)GeTe.. *Science Advances*, **2022**, 8, eabm7103	10.3	10
47	Methane storage capabilities of diamond analogues. *Physical Chemistry Chemical Physics*, **2013**, 15, 20937-42	3.4	9
46	Energy level alignment of self-assembled linear chains of benzenediamine on Au(111) from first principles. *Physical Review B*, **2016**, 93,	3.3	8
45	Effects of quantum confinement on excited state properties of SrTiO3 from ab initio many-body perturbation theory. *Physical Review B*, **2016**, 94,	3.3	8
44	Anisotropic 2D excitons unveiled in organic-inorganic quantum wells. *Materials Horizons*, **2021**, 8, 197-208	14.4	8
43	Anisotropic Dirac Fermions in BaMnBi and BaZnBi. *Scientific Reports*, **2018**, 8, 15322	4.9	8
42	Band gaps of crystalline solids from Wannier-localization-based optimal tuning of a screened range-separated hybrid functional. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	8
41	First-Principles Approach to the Conductance of Covalently Bound Molecular Junctions. *Journal of Physical Chemistry C*, **2019**, 123, 6379-6387	3.8	7
40	Tuning the electronic structure of SrTiO3/SrFeO3 superlattices via composition and vacancy control. *APL Materials*, **2014**, 2, 046101	5.7	7
39	. *Computing in Science and Engineering*, **2010**, 12, 18-27	1.5	7
38	The energy level alignment at metal molecule interfaces using Wannier Koopmans method. *Applied Physics Letters*, **2016**, 108, 262104	3.4	7
37	Reduced scaling formulation of CASPT2 analytical gradients using the supporting subspace method. *Journal of Chemical Physics*, **2021**, 154, 014103	3.9	7
36	Algorithm for efficient elastic transport calculations for arbitrary device geometries. *Physical Review B*, **2011**, 84,	3.3	6
35	Ferroelectricity in [111]-oriented epitaxially strained SrTiO3 from first principles. *Physical Review Materials*, **2019**, 3,	3.2	6
34	Band gap renormalization, carrier mobilities, and the electron-phonon self-energy in crystalline naphthalene. *Physical Review B*, **2020**, 101,	3.3	5
33	First-principles studies of proton-Ba interactions in doped LaPO4. *Journal of Materials Chemistry*, **2012**, 22, 3758		5
32	From the interface energy to the solubility limit of aluminium in nickel from first-principles and Kinetic Monte Carlo calculations. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **2011**, 176, 767-771	3.1	5
31	Topological semimetal features in the multiferroic hexagonal manganites. *Physical Review Materials*, **2019**, 3,	3.2	5

30	Cooperative Carbon Dioxide Adsorption in Alcoholamine- and Alkoxyalkylamine-Functionalized Metal□Organic Frameworks. *Angewandte Chemie*, **2020**, 132, 19636-19645	3.6	4
29	Adsorption and Stability of □Bonded Ethylene on GaP(110). *Journal of Physical Chemistry C*, **2013**, 117, 26091-26096	3.8	4
28	Pressure amorphization through displacive disorder. *European Physical Journal E*, **2002**, 9, 239-43	1.5	4
27	Band Edge Tailoring in Few-Layer Two-Dimensional Molybdenum Sulfide/Selenide Alloys. *Journal of Physical Chemistry C*, **2020**, 124, 22893-22902	3.8	4
26	Signatures of possible surface states in TaAs. *Physical Review B*, **2020**, 102,	3.3	4
25	Phonon Screening of Excitons in Semiconductors: Halide Perovskites and Beyond. *Physical Review Letters*, **2021**, 127, 067401	7.4	4
24	Emergence of topological electronic phases in elemental lithium under pressure. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 9197-9201	11.5	3
23	Dehydrogenation of Ammonia on Ru(0001) by Electronic Excitations. *Journal of Physical Chemistry C* , **2015**, 119, 10520-10525	3.8	3
22	Covalent Functionalization of GaP(110) Surfaces via a Staudinger-Type Reaction with Perfluorophenyl Azide. *Journal of Physical Chemistry C*, **2016**, 120, 26448-26452	3.8	3
21	Superlattice-induced ferroelectricity in charge-ordered LaSrFeO. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 23972-23976	11.5	3
20	Elucidating heterogeneity in nanoplasmonic structures using nonlinear photon localization microscopy. *Journal of Optics (United Kingdom)*, **2014**, 16, 114014	1.7	3
19	Evolution of the Interfacial Electronic Structure During Thermal Oxidation. *Springer Series in Materials Science*, **2001**, 219-246	0.9	3
18	Push it to the limit: comparing periodic and local approaches to density functional theory for intermolecular interactions. *Molecular Physics*, **2019**, 117, 1298-1305	1.7	3
17	Resonance Raman Characterization of Tetracene Monomer and Nanocrystals: Excited State Lattice Distortions With Implications For Efficient Singlet Fission. *Journal of Physical Chemistry A*, **2019**, 123, 3863-3875	2.8	2
16	Prediction of TiRhAs as a Dirac nodal line semimetal via first-principles calculations. *Physical Review B*, **2017**, 96,	3.3	2
15	Interfacing carbon nanotubes of arbitrary chiralities into linear heterojunctions. *Physical Review B*, **2011**, 83,	3.3	2
14	Publisher□s Note: Ab initio study of the phase diagram of epitaxial BaTiO3 [Phys. Rev. B 69, 212101 (2004)]. *Physical Review B*, **2004**, 70,	3.3	2
13	Half-magnetization plateau and the origin of threefold symmetry breaking in an electrically switchable triangular antiferromagnet. *Physical Review Research*, **2020**, 2,	3.9	2

List of Publications

12	Time-Dependent Density Functional Theory of Narrow Band Gap Semiconductors Using a Screened Range-Separated Hybrid Functional. *Advanced Theory and Simulations*, **2020**, 3, 2000220	3.5	2
11	Gold-Cage Perovskites: A Three-Dimensional Au-X Framework Encasing Isolated MX Octahedra (M = In, Sb, Bi; X = Cl, Br, I). *Journal of the American Chemical Society*, **2021**, 143, 7440-7448	16.4	2
10	Origins of anisotropic transport in the electrically switchable antiferromagnet Fe1/3NbS2. *Physical Review B*, **2021**, 103,	3.3	2
9	Density of states prediction for materials discovery via contrastive learning from probabilistic embeddings.. *Nature Communications*, **2022**, 13, 949	17.4	2
8	High Compression-Induced Conductivity in a Layered CuBr Perovskite. *Angewandte Chemie*, **2020**, 132, 4046-4051	3.6	1
7	Expanded Analogs of Three-Dimensional Lead-Halide Hybrid Perovskites. *Angewandte Chemie*, **2020**, 132, 19249-19256	3.6	1
6	Band Edge Energy Tuning through Electronic Character Hybridization in Ternary Metal Vanadates. *Chemistry of Materials*, **2021**, 33, 7242-7253	9.6	1
5	Alkaline-stable nickel manganese oxides with ideal band gap for solar fuel photoanodes. *Chemical Communications*, **2018**, 54, 4625-4628	5.8	0
4	Accelerated Discovery of CH 4 Uptake Capacity Metal-Organic Frameworks Using Bayesian Optimization. *Advanced Theory and Simulations*,2100515	3.5	0
3	A diagrammatic approach for automatically deriving analytical gradients of tensor hyper-contracted electronic structure methods. *Journal of Chemical Physics*, **2021**, 155, 024108	3.9	0
2	Exchange Bias in a Layered Metal-Organic Topological Spin Glass. *ACS Central Science*, **2021**, 7, 1317-1326	16.8	0
1	An assessment of density functionals for predicting CO adsorption in diamine-functionalized metal-organic frameworks.. *Journal of Chemical Physics*, **2022**, 156, 154113	3.9	0