Leeor Kronik

List of Publications by Year in Descending Order

247 papers	18,474 citations	67 h-index	130 g-index
265 ext. papers	20,303 ext. citations	7.5 avg, IF	7.11 L-index

#	Paper	IF	Citations
247	Theory of Chirality Induced Spin Selectivity: Progress and Challenges.. *Advanced Materials*, **2022**, e2106629	24	14
246	Single Excitation Energies Obtained from the Ensemble "HOMO-LUMO Gap": Exact Results and Approximations.. *Journal of Physical Chemistry Letters*, **2022**, 2452-2458	6.4	0
245	Optimal Tuning Perspective of Range-Separated Double Hybrid Functionals.. *Journal of Chemical Theory and Computation*, **2022**, 18, 2331-2340	6.4	1
244	Real-space crystal structure analysis by low-dose focal-series TEM imaging of organic materials with near-atomic resolution.. *Advanced Materials*, **2022**, e2202088	24	0
243	Anisotropic Interlayer Force Field for Transition Metal Dichalcogenides: The Case of Molybdenum Disulfide. *Journal of Chemical Theory and Computation*, **2021**, 17, 7237-7245	6.4	3
242	Hydrogen freedom linked to perovskite efficiency. *Nature Materials*, **2021**, 20, 914-915	27	
241	Mechanism and Timescales of Reversible p-Doping of Methylammonium Lead Triiodide by Oxygen. *Advanced Materials*, **2021**, 33, e2100211	24	8
240	Generalized Heisenberg-Type Magnetic Phenomena in Coordination Polymers with Nickel–Lanthanide Dinuclear Units. *Journal of Physical Chemistry C*, **2021**, 125, 11182-11196	3.8	4
239	Space-Filling Curves for Real-Space Electronic Structure Calculations. *Journal of Chemical Theory and Computation*, **2021**, 17, 4039-4048	6.4	1
238	The pursuit of stability in halide perovskites: the monovalent cation and the key for surface and bulk self-healing. *Materials Horizons*, **2021**, 8, 1570-1586	14.4	5
237	Quantitative explanation of the Schottky barrier height. *Physical Review B*, **2021**, 103,	3.3	6
236	Ensemble generalized Kohn-Sham theory: The good, the bad, and the ugly. *Journal of Chemical Physics*, **2021**, 154, 094125	3.9	8
235	Double excitations in molecules from ensemble density functionals: Theory and approximations. *Physical Review A*, **2021**, 104,	2.6	4
234	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
233	Exact Generalized Kohn-Sham Theory for Hybrid Functionals. *Physical Review X*, **2020**, 10,	9.1	10
232	General Approach for Reducing Continuous Translational Symmetry Errors in Finite Difference Real-Space Calculations. *Journal of Chemical Theory and Computation*, **2020**, 16, 4327-4336	6.4	
231	Piecewise linearity, freedom from self-interaction, and a Coulomb asymptotic potential: three related yet inequivalent properties of the exact density functional. *Physical Chemistry Chemical Physics*, **2020**, 22, 16467-16481	3.6	16

230	Assessment of the Performance of Optimally Tuned Range-Separated Hybrid Functionals for Nuclear Magnetic Shielding Calculations. *Advanced Theory and Simulations*, **2020**, 3, 2000083	3.5	2
229	Fe-porphyrin on Co(001) and Cu(001): A Comparative Dispersion-augmented Density Functional Theory Study. *Israel Journal of Chemistry*, **2020**, 60, 870-875	3.4	
228	Role of long-range exact exchange in polaron charge transition levels: The case of MgO. *Physical Review Materials*, **2020**, 4,	3.2	3
227	Order and Disorder in Calcium Oxalate Monohydrate: Insights from First-Principles Calculations. *Crystal Growth and Design*, **2020**, 20, 858-865	3.5	2
226	Mechanical and Tribological Properties of Layered Materials under High Pressure: Assessing the Importance of Many-Body Dispersion Effects. *Journal of Chemical Theory and Computation*, **2020**, 16, 666-676	6.4	19
225	Long-Range Spin-Selective Transport in Chiral Metal-Organic Crystals with Temperature-Activated Magnetization. *ACS Nano*, **2020**,	16.7	22
224	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
223	Asymptotic behavior of the Hartree-exchange and correlation potentials in ensemble density functional theory. *Physical Chemistry Chemical Physics*, **2019**, 21, 19805-19815	3.6	13
222	Structure and Morphology of Light-Reflecting Synthetic and Biogenic Polymorphs of Isoxanthopterin: A Comparison. *Chemistry of Materials*, **2019**, 31, 4479-4489	9.6	7
221	Bulklike band-offset mystery solved through energy minimization: Lessons from perovskite oxide heterojunctions. *Physical Review B*, **2019**, 99,	3.3	5
220	Accurate Magnetic Couplings in Chromium-Based Molecular Rings from Broken-Symmetry Calculations within Density Functional Theory. *Journal of Chemical Theory and Computation*, **2019**, 15, 4885-4895	6.4	2
219	Breakdown of the Static Picture of Defect Energetics in Halide Perovskites: The Case of the Br Vacancy in CsPbBr. *Journal of Physical Chemistry Letters*, **2019**, 10, 4490-4498	6.4	25
218	Spatial Phase Distributions in Solution-Based and Evaporated $CsPbBr_3$ Thin Films. *Journal of Physical Chemistry C*, **2019**, 123, 17666-17677	3.8	8
217	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
216	Transferable screened range-separated hybrids for layered materials: The cases of MoS2 and h-BN. *Physical Review Materials*, **2019**, 3,	3.2	10
215	Magnetic configurations of open-shell molecules on metals: The case of CuPc and CoPc on silver. *Physical Review Materials*, **2019**, 3,	3.2	2
214	Systematic modification of the indium tin oxide work function via side-chain modulation of an amino-acid functionalization layer. *Physical Chemistry Chemical Physics*, **2019**, 21, 21875-21881	3.6	4
213	Mechanically rigid supramolecular assemblies formed from an Fmoc-guanine conjugated peptide nucleic acid. *Nature Communications*, **2019**, 10, 5256	17.4	9

212	Guanine and 7,8-Dihydroxanthopterin Reflecting Crystals in the Zander Fish Eye: Crystal Locations, Compositions, and Structures. *Journal of the American Chemical Society*, **2019**, 141, 19736-19745	16.4	10
211	Nonmagnetic single-molecule spin-filter based on quantum interference. *Nature Communications*, **2019**, 10, 5565	17.4	32
210	Constructing the Electronic Structure of CHNHPbI and CHNHPbBr Perovskite Thin Films from Single-Crystal Band Structure Measurements. *Journal of Physical Chemistry Letters*, **2019**, 10, 601-609	6.4	55
209	Optically functional isoxanthopterin crystals in the mirrored eyes of decapod crustaceans. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 2299-2304	11.5	28
208	Molecule-Adsorbed Topological Insulator and Metal Surfaces: A Comparative First-Principles Study. *Chemistry of Materials*, **2018**, 30, 1849-1855	9.6	6
207	Dielectric Screening Meets Optimally Tuned Density Functionals. *Advanced Materials*, **2018**, 30, e1706560	24	76
206	Electronic structure of dipeptides in the gas-phase and as an adsorbed monolayer. *Physical Chemistry Chemical Physics*, **2018**, 20, 6860-6867	3.6	8
205	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
204	Effect of Internal Heteroatoms on Level Alignment at Metal/Molecular Monolayer/Si Interfaces. *Journal of Physical Chemistry C*, **2018**, 122, 3312-3325	3.8	6
203	Charge transfer excitations from exact and approximate ensemble Kohn-Sham theory. *Journal of Chemical Physics*, **2018**, 148, 174101	3.9	23
202	What Remains Unexplained about the Properties of Halide Perovskites?. *Advanced Materials*, **2018**, 30, e1800691	24	174
201	The effect of ionic composition on acoustic phonon speeds in hybrid perovskites from Brillouin spectroscopy and density functional theory. *Journal of Materials Chemistry C*, **2018**, 6, 3861-3868	7.1	17
200	Time-dependent generalized Kohn-Sham theory. *European Physical Journal B*, **2018**, 91, 1	1.2	60
199	Separation of enantiomers by their enantiospecific interaction with achiral magnetic substrates. *Science*, **2018**, 360, 1331-1334	33.3	183
198	Terahertz spectroscopy of 2,4,6-trinitrotoluene molecular solids from first principles. *Beilstein Journal of Organic Chemistry*, **2018**, 14, 381-388	2.5	6
197	Bioinspired Flexible and Tough Layered Peptide Crystals. *Advanced Materials*, **2018**, 30, 1704551	24	17
196	Charge Density and Band Offsets at Heterovalent Semiconductor Interfaces. *Advanced Theory and Simulations*, **2018**, 1, 1700001	3.5	12
195	Vibrational properties of isotopically enriched materials: the case of calcite.. *RSC Advances*, **2018**, 8, 33985-33992	3.7	4

194	Fundamental Gaps of Condensed-Phase Organic Semiconductors from Single-Molecule Calculations using Polarization-Consistent Optimally Tuned Screened Range-Separated Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2018**, 14, 6287-6294	6.4	52
193	Photoelectron spectra of copper oxide cluster anions from first principles methods. *Journal of Chemical Physics*, **2018**, 149, 064306	3.9	5
192	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
191	Prediction of electronic couplings for molecular charge transfer using optimally tuned range-separated hybrid functionals. *Molecular Physics*, **2018**, 116, 2497-2505	1.7	12
190	Spin-State Energetics of Fe Complexes from an Optimally Tuned Range-Separated Hybrid Functional. *Chemistry - A European Journal*, **2018**, 24, 5173-5182	4.8	24
189	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
188	Biologically Controlled Morphology and Twinning in Guanine Crystals. *Angewandte Chemie - International Edition*, **2017**, 56, 9420-9424	16.4	25
187	Local Polar Fluctuations in Lead Halide Perovskite Crystals. *Physical Review Letters*, **2017**, 118, 136001	7.4	374
186	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
185	Light-induced picosecond rotational disordering of the inorganic sublattice in hybrid perovskites. *Science Advances*, **2017**, 3, e1602388	14.3	109
184	Interlayer Potential for Homogeneous Graphene and Hexagonal Boron Nitride Systems: Reparametrization for Many-Body Dispersion Effects. *Journal of Physical Chemistry C*, **2017**, 121, 22826-22835	3.8	37
183	Biologically Controlled Morphology and Twinning in Guanine Crystals. *Angewandte Chemie*, **2017**, 129, 9548-9552	3.6	4
182	Valence electronic structure of cobalt phthalocyanine from an optimally tuned range-separated hybrid functional. *Journal of Chemical Physics*, **2017**, 147, 044301	3.9	39
181	Effect of Solid-State Polarization on Charge-Transfer Excitations and Transport Levels at Organic Interfaces from a Screened Range-Separated Hybrid Functional. *Journal of Physical Chemistry Letters*, **2017**, 8, 3277-3283	6.4	55
180	Band offset formation at semiconductor heterojunctions through density-based minimization of interface energy. *Physical Review B*, **2016**, 94,	3.3	13
179	Tuning electronic transport via hepta-alanine peptides junction by tryptophan doping. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 10785-90	11.5	57
178	Structural and excited-state properties of oligoacene crystals from first principles. *Physical Review B*, **2016**, 93,	3.3	73
177	Hybrid organic–inorganic perovskites: low-cost semiconductors with intriguing charge-transport properties. *Nature Reviews Materials*, **2016**, 1,	73.3	912

176	Driven Liouville von Neumann Approach for Time-Dependent Electronic Transport Calculations in a Nonorthogonal Basis-Set Representation. *Journal of Physical Chemistry C*, **2016**, 120, 15052-15062	3.8	20
175	Hybrid Organic-Inorganic Perovskites on the Move. *Accounts of Chemical Research*, **2016**, 49, 573-81	24.3	176
174	Ionisation and (de-)protonation energies of gas-phase amino acids from an optimally tuned range-separated hybrid functional. *Molecular Physics*, **2016**, 114, 1218-1224	1.7	8
173	Interplay of Bias-Driven Charging and the Vibrational Stark Effect in Molecular Junctions. *Nano Letters*, **2016**, 16, 1104-9	11.5	32
172	Enhanced Magnetoresistance in Molecular Junctions by Geometrical Optimization of Spin-Selective Orbital Hybridization. *Nano Letters*, **2016**, 16, 1741-5	11.5	30
171	Valence and Conduction Band Densities of States of Metal Halide Perovskites: A Combined Experimental-Theoretical Study. *Journal of Physical Chemistry Letters*, **2016**, 7, 2722-9	6.4	264
170	Real-space pseudopotential method for computing the vibrational Stark effect. *Journal of Chemical Physics*, **2016**, 145, 174111	3.9	3
169	Origin and structure of polar domains in doped molecular crystals. *Nature Communications*, **2016**, 7, 13351	17.4	24
168	Cold denaturation induces inversion of dipole and spin transfer in chiral peptide monolayers. *Nature Communications*, **2016**, 7, 10744	17.4	62
167	Excited-State Properties of Molecular Solids from First Principles. *Annual Review of Physical Chemistry*, **2016**, 67, 587-616	15.7	64
166	High Chloride Doping Levels Stabilize the Perovskite Phase of Cesium Lead Iodide. *Nano Letters*, **2016**, 16, 3563-70	11.5	208
165	Interlayer Potential for Graphene/h-BN Heterostructures. *Journal of Chemical Theory and Computation*, **2016**, 12, 2896-905	6.4	69
164	Optical phonons in methylammonium lead halide perovskites and implications for charge transport. *Materials Horizons*, **2016**, 3, 613-620	14.4	228
163	Multiscale approach to the electronic structure of doped semiconductor surfaces. *Physical Review B* , **2015**, 91,	3.3	24
162	Deviations from piecewise linearity in the solid-state limit with approximate density functionals. *Journal of Chemical Physics*, **2015**, 142, 034107	3.9	36
161	Electronic Transport via Homopeptides: The Role of Side Chains and Secondary Structure. *Journal of the American Chemical Society*, **2015**, 137, 9617-26	16.4	81
160	Elimination of the asymptotic fractional dissociation problem in Kohn-Sham density-functional theory using the ensemble-generalization approach. *Physical Review A*, **2015**, 91,	2.6	24
159	Reliable energy level alignment at physisorbed molecule-metal interfaces from density functional theory. *Nano Letters*, **2015**, 15, 2448-55	11.5	88

158	Molecule-lead coupling at molecular junctions: relation between the real- and state-space perspectives. *Journal of Chemical Theory and Computation*, **2015**, 11, 4861-9	6.4	23
157	Effect of binding group on hybridization across the silicon/aromatic-monolayer interface. *Journal of Electron Spectroscopy and Related Phenomena*, **2015**, 204, 149-158	1.7	7
156	Are Mobilities in Hybrid Organic-Inorganic Halide Perovskites Actually "High"?. *Journal of Physical Chemistry Letters*, **2015**, 6, 4754-7	6.4	167
155	Relating the Physical Structure and Optoelectronic Function of Crystalline TIPS-Pentacene. *Advanced Functional Materials*, **2015**, 25, 2038-2046	15.6	64
154	Theory of Hydrogen Migration in Organic□Inorganic Halide Perovskites. *Angewandte Chemie*, **2015**, 127, 12614-12618	3.6	7
153	Solid-state optical absorption from optimally tuned time-dependent range-separated hybrid density functional theory. *Physical Review B*, **2015**, 92,	3.3	171
152	Effect of ensemble generalization on the highest-occupied Kohn-Sham eigenvalue. *Journal of Chemical Physics*, **2015**, 143, 104105	3.9	13
151	Unusually Large Young's Moduli of Amino Acid Molecular Crystals. *Angewandte Chemie - International Edition*, **2015**, 54, 13566-70	16.4	54
150	Hybrid Organic-Inorganic Perovskites (HOIPs): Opportunities and Challenges. *Advanced Materials*, **2015**, 27, 5102-12	24	325
149	Unusually Large Young□ Moduli of Amino Acid Molecular Crystals. *Angewandte Chemie*, **2015**, 127, 13770-13774	3.6	9
148	Theory of hydrogen migration in organic-inorganic halide perovskites. *Angewandte Chemie - International Edition*, **2015**, 54, 12437-41	16.4	112
147	□uanigma□The Revised Structure of Biogenic Anhydrous Guanine. *Chemistry of Materials*, **2015**, 27, 8289-8297	9.6	47
146	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
145	Infrared Absorption Spectrum of Brushite from First Principles. *Chemistry of Materials*, **2014**, 26, 2934-2942	9.6	34
144	Gas-phase valence-electron photoemission spectroscopy using density functional theory. *Topics in Current Chemistry*, **2014**, 347, 137-91		35
143	One-electron self-interaction and the asymptotics of the Kohn-Sham potential: an impaired relation. *Physical Chemistry Chemical Physics*, **2014**, 16, 14357-67	3.6	46
142	State Representation Approach for Atomistic Time-Dependent Transport Calculations in Molecular Junctions. *Journal of Chemical Theory and Computation*, **2014**, 10, 2927-41	6.4	44
141	Why are diphenylalanine-based peptide nanostructures so rigid? Insights from first principles calculations. *Journal of the American Chemical Society*, **2014**, 136, 963-9	16.4	115

140	Role of Dispersive Interactions in Determining Structural Properties of Organic-Inorganic Halide Perovskites: Insights from First-Principles Calculations. *Journal of Physical Chemistry Letters*, **2014**, 5, 2728-33	6.4	168
139	Experimental and theoretical electronic structure of quinacridone. *Physical Review B*, **2014**, 90,	3.3	56
138	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
137	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
136	Probing the orbital origin of conductance oscillations in atomic chains. *Nano Letters*, **2014**, 14, 2988-93	11.5	17
135	Understanding molecular crystals with dispersion-inclusive density functional theory: pairwise corrections and beyond. *Accounts of Chemical Research*, **2014**, 47, 3208-16	24.3	121
134	Fundamental gaps with approximate density functionals: the derivative discontinuity revealed from ensemble considerations. *Journal of Chemical Physics*, **2014**, 140, 18A540	3.9	58
133	Real-space method for highly parallelizable electronic transport calculations. *Physical Review B*, **2014**, 90,	3.3	7
132	Inter-layer potential for hexagonal boron nitride. *Journal of Chemical Physics*, **2014**, 140, 104106	3.9	49
131	A self-interaction-free local hybrid functional: accurate binding energies vis-à-vis accurate ionization potentials from Kohn-Sham eigenvalues. *Journal of Chemical Physics*, **2014**, 140, 18A510	3.9	50
130	Effect of Molecule-Surface Reaction Mechanism on the Electronic Characteristics and Photovoltaic Performance of Molecularly Modified Si. *Journal of Physical Chemistry C*, **2013**, 117, 22351-22361	3.8	21
129	Electronic structure of CoPc adsorbed on Ag(100): Evidence for molecule-substrate interaction mediated by Co 3d orbitals. *Physical Review B*, **2013**, 87,	3.3	49
128	Gap renormalization of molecular crystals from density-functional theory. *Physical Review B*, **2013**, 88,	3.3	197
127	Using optimally tuned range separated hybrid functionals in ground-state calculations: consequences and caveats. *Journal of Chemical Physics*, **2013**, 138, 204115	3.9	140
126	Locally Refined Multigrid Solution of the All-Electron Kohn-Sham Equation. *Journal of Chemical Theory and Computation*, **2013**, 9, 4744-60	6.4	10
125	Understanding the Metal–Molecule Interface from First Principles **2013**, 51-89		9
124	Effect of Doping Density on the Charge Rearrangement and Interface Dipole at the Molecule–Silicon Interface. *Journal of Physical Chemistry C*, **2013**, 117, 22422-22427	3.8	12
123	Atomically wired molecular junctions: connecting a single organic molecule by chains of metal atoms. *Nano Letters*, **2013**, 13, 1956-61	11.5	43

122	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
121	Pair-Wise and Many-Body Dispersive Interactions Coupled to an Optimally Tuned Range-Separated Hybrid Functional. *Journal of Chemical Theory and Computation*, **2013**, 9, 3473-8	6.4	20
120	Piecewise linearity of approximate density functionals revisited: implications for frontier orbital energies. *Physical Review Letters*, **2013**, 110, 126403	7.4	97
119	Simulated doping of Si from first principles using pseudoatoms. *Physical Review B*, **2013**, 87,	3.3	13
118	Curvature and Frontier Orbital Energies in Density Functional Theory. *Journal of Physical Chemistry Letters*, **2012**, 3, 3740-4	6.4	134
117	Hybrids of organic molecules and flat, oxide-free silicon: high-density monolayers, electronic properties, and functionalization. *Langmuir*, **2012**, 28, 9920-9	4	98
116	Dimensionality effects in the electronic structure of organic semiconductors consisting of polar repeat units. *Organic Electronics*, **2012**, 13, 3165-3176	3.5	19
115	Quasiparticle spectra from a nonempirical optimally tuned range-separated hybrid density functional. *Physical Review Letters*, **2012**, 109, 226405	7.4	203
114	Quasiparticle and optical spectroscopy of the organic semiconductors pentacene and PTCDA from first principles. *Physical Review B*, **2012**, 85,	3.3	158
113	Magnetic Properties of Fe/Cu Codoped ZnO Nanocrystals. *Journal of Physical Chemistry Letters*, **2012**, 3, 2009-2014	6.4	34
112	Excitation Gaps of Finite-Sized Systems from Optimally Tuned Range-Separated Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2012**, 8, 1515-31	6.4	642
111	Charge transport across metal/molecular (alkyl) monolayer-Si junctions is dominated by the LUMO level. *Physical Review B*, **2012**, 85,	3.3	48
110	Electronic level alignment at a metal-molecule interface from a short-range hybrid functional. *Journal of Chemical Physics*, **2011**, 135, 164706	3.9	65
109	Collectively induced quantum-confined Stark effect in monolayers of molecules consisting of polar repeating units. *Journal of the American Chemical Society*, **2011**, 133, 18634-45	16.4	31
108	Electronic structure of copper phthalocyanine from G0W0 calculations. *Physical Review B*, **2011**, 84,	3.3	80
107	Fundamental and excitation gaps in molecules of relevance for organic photovoltaics from an optimally tuned range-separated hybrid functional. *Physical Review B*, **2011**, 84,	3.3	252
106	Dispersion Interactions with Density-Functional Theory: Benchmarking Semiempirical and Interatomic Pairwise Corrected Density Functionals. *Journal of Chemical Theory and Computation*, **2011**, 7, 3944-51	6.4	230
105	Decoupling local disorder and optical effects in infrared spectra: differentiating between calcites with different origins. *Advanced Materials*, **2011**, 23, 550-4	24	72

104	Role of Backbone Charge Rearrangement in the Bond-Dipole and Work Function of Molecular Monolayers. *Journal of Physical Chemistry C*, **2011**, 115, 24888-24892	3.8	28
103	Charge-Transfer-Like π→π* Excitations in Time-Dependent Density Functional Theory: A Conundrum and Its Solution. *Journal of Chemical Theory and Computation*, **2011**, 7, 2408-15	6.4	204
102	Fully Numerical All-Electron Solutions of the Optimized Effective Potential Equation for Diatomic Molecules. *Journal of Chemical Theory and Computation*, **2011**, 7, 2665	6.4	6
101	Structure and Formation of Synthetic Hemozoin: Insights From First-Principles Calculations. *Crystal Growth and Design*, **2011**, 11, 3332-3341	3.5	32
100	Dissociation of diatomic molecules and the exact-exchange Kohn-Sham potential: The case of LiF. *Physical Review A*, **2011**, 83,	2.6	34
99	Electronic Properties of Organic-Based Interfaces. *MRS Bulletin*, **2010**, 35, 417-421	3.2	42
98	Stacking and registry effects in layered materials: the case of hexagonal boron nitride. *Physical Review Letters*, **2010**, 105, 046801	7.4	256
97	Describing Both Dispersion Interactions and Electronic Structure Using Density Functional Theory: The Case of Metal-Phthalocyanine Dimers. *Journal of Chemical Theory and Computation*, **2010**, 6, 81-90	6.4	100
96	Hg/Molecular Monolayer/Si Junctions: Electrical Interplay between Monolayer Properties and Semiconductor Doping Density. *Journal of Physical Chemistry C*, **2010**, 114, 10270-10279	3.8	51
95	Fundamental gaps in finite systems from eigenvalues of a generalized Kohn-Sham method. *Physical Review Letters*, **2010**, 105, 266802	7.4	338
94	Polarizability, Susceptibility, and Dielectric Constant of Nanometer-Scale Molecular Films: A Microscopic View. *Advanced Functional Materials*, **2010**, 20, 2077-2084	15.6	47
93	Examining the role of pseudopotentials in exact-exchange-based Kohn-Sham gaps. *Physical Review B*, **2009**, 80,	3.3	14
92	Density functional theory of transition metal phthalocyanines, II: electronic structure of MnPc and FePc/symmetry and symmetry breaking. *Applied Physics A: Materials Science and Processing*, **2009**, 95, 165-172	2.6	95
91	Density functional theory of transition metal phthalocyanines, I: electronic structure of NiPc and CoPc/self-interaction effects. *Applied Physics A: Materials Science and Processing*, **2009**, 95, 159-163	2.6	101
90	Real-space pseudopotential method for noncollinear magnetism within density functional theory. *Solid State Communications*, **2009**, 149, 177-180	1.6	7
89	Fully Numerical All-Electron Solutions of the Optimized Effective Potential Equation for Diatomic Molecules. *Journal of Chemical Theory and Computation*, **2009**, 5, 1731-40	6.4	37
88	The molecularly controlled semiconductor resistor: how does it work?. *ACS Applied Materials & Interfaces*, **2009**, 1, 2679-83	9.5	19
87	Cooperative effects in molecular conduction II: The semiconductor-metal molecular junction. *Journal of Physical Chemistry A*, **2009**, 113, 7451-60	2.8	15

86	When to trust photoelectron spectra from Kohn-Sham eigenvalues: The case of organic semiconductors. *Physical Review B*, **2009**, 79,	3.3	96
85	Prediction of charge-transfer excitations in coumarin-based dyes using a range-separated functional tuned from first principles. *Journal of Chemical Physics*, **2009**, 131, 244119	3.9	270
84	Reliable prediction of charge transfer excitations in molecular complexes using time-dependent density functional theory. *Journal of the American Chemical Society*, **2009**, 131, 2818-20	16.4	632
83	Electronic structure of copper phthalocyanine: a comparative density functional theory study. *Journal of Chemical Physics*, **2008**, 128, 164107	3.9	143
82	Defect-Dominated Charge Transport in Si-Supported CdSe Nanoparticle Films. *Journal of Physical Chemistry C*, **2008**, 112, 6564-6570	3.8	15
81	Electronic Characterization of Si(100)-Bound Alkyl Monolayers Using Kelvin Probe Force Microscopy. *Journal of Physical Chemistry C*, **2008**, 112, 7145-7150	3.8	27
80	A New "Bottom-Up" Framework for Teaching Chemical Bonding. *Journal of Chemical Education*, **2008**, 85, 1680	2.4	28
79	Integrated circuits based on nanoscale vacuum phototubes. *Applied Physics Letters*, **2008**, 92, 262903	3.4	14
78	Real-space pseudopotential method for first principles calculations of general periodic and partially periodic systems. *Physical Review B*, **2008**, 78,	3.3	66
77	Orbital-dependent density functionals: Theory and applications. *Reviews of Modern Physics*, **2008**, 80, 3-60	40.5	941
76	Cooperative Effects in Molecular Conduction. *Journal of Computational and Theoretical Nanoscience* , **2008**, 5, 535-544	0.3	35
75	Polarizability of small carbon cluster anions from first principles. *Journal of Physical Chemistry A*, **2007**, 111, 2028-32	2.8	13
74	Tangential ligand-induced strain in icosahedral Au13. *Journal of the American Chemical Society*, **2007**, 129, 10978-9	16.4	28
73	Electrostatic properties of adsorbed polar molecules: opposite behavior of a single molecule and a molecular monolayer. *Journal of the American Chemical Society*, **2007**, 129, 2989-97	16.4	57
72	Local atomic order and infrared spectra of biogenic calcite. *Angewandte Chemie - International Edition*, **2007**, 46, 291-4	16.4	57
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