Leeor Kronik

List of Publications by Year
in descending order

249	22,237	8755 75	9589 142
papers	citations	h-index	g-index

265	265	265	19848
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Theory of Chirality Induced Spin Selectivity: Progress and Challenges. Advanced Materials, 2022, 34, e2106629.	21.0	119
2	Adiabatic Connection for Rangeâ€Separated Hybrid Functionals. Advanced Theory and Simulations, 2022, 5, .	2.8	1
3	Electronic Structure, Bonding, and Stability of Boron Subphthalocyanine Halides and Pseudohalides. Advanced Theory and Simulations, 2022, 5, .	2.8	8
4	Single Excitation Energies Obtained from the Ensemble â€œHOMOâ€“LUMO Gapâ€: Exact Results and Approximations. Journal of Physical Chemistry Letters, 2022, 13, 2452-2458.	4.6	14
5	Polymorphism, Structure, and Nucleation of CholesterolÂ·H₂O at Aqueous Interfaces and in Pathological Media: Revisited from a Computational Perspective. Journal of the American Chemical Society, 2022, 144, 5304-5314.	13.7	8
6	Optimal Tuning Perspective of Range-Separated Double Hybrid Functionals. Journal of Chemical Theory and Computation, 2022, 18, 2331-2340.	5.3	6
7	Realâ€Space Crystal Structure Analysis by Lowâ€Dose Focalâ€Series TEM Imaging of Organic Materials with Nearâ€Atomic Resolution. Advanced Materials, 2022, 34, e2202088.	21.0	4
8	Optimally tuned starting point for single-shot<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m of solids. Physical Review Materials, 2022, 6, .	2.4	11
9	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.	12.2	29
10	Quantitative explanation of the Schottky barrier height. Physical Review B, 2021, 103, .	3.2	10
11	Fermi level pinning for zinc-blende semiconductors explained with interface bonds. Physical Review B, 2021, 103, .	3.2	7
12	Ensemble generalized Kohnâ€“Sham theory: The good, the bad, and the ugly. Journal of Chemical Physics, 2021, 154, 094125.	3.0	12
13	Hydrogen freedom linked to perovskite efficiency. Nature Materials, 2021, 20, 914-915.	27.5	1
14	Mechanism and Timescales of Reversible pâ€Doping of Methylammonium Lead Triiodide by Oxygen. Advanced Materials, 2021, 33, e2100211.	21.0	17
15	Generalized Heisenberg-Type Magnetic Phenomena in Coordination Polymers with Nickelâ€“Lanthanide Dinuclear Units. Journal of Physical Chemistry C, 2021, 125, 11182-11196.	3.1	7
16	Space-Filling Curves for Real-Space Electronic Structure Calculations. Journal of Chemical Theory and Computation, 2021, 17, 4039-4048.	5.3	11
17	Double excitations in molecules from ensemble density functionals: Theory and approximations. Physical Review A, 2021, 104, .	2.5	10
18	Band gaps of crystalline solids from Wannier-localizationâ€“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, .	7.1	49

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19	Are Defects in Lead-Halide Perovskites Healed, Tolerated, or Both?. ACS Energy Letters, 2021, 6, 4108-4114.	17.4	31
20	Anisotropic Interlayer Force Field for Transition Metal Dichalcogenides: The Case of Molybdenum Disulfide. Journal of Chemical Theory and Computation, 2021, 17, 7237-7245.	5.3	12
21	Order and Disorder in Calcium Oxalate Monohydrate: Insights from First-Principles Calculations. Crystal Growth and Design, 2020, 20, 858-865.	3.0	5
22	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.	5.3	39
23	Long-Range Spin-Selective Transport in Chiral Metalâ€“Organic Crystals with Temperature-Activated Magnetization. ACS Nano, 2020, 14, 16624-16633.	14.6	51
24	Timeâ€Dependent Density Functional Theory of Narrow Band Gap Semiconductors Using a Screened Rangeâ€Separated Hybrid Functional. Advanced Theory and Simulations, 2020, 3, 2000220.	2.8	6
25	Exact Generalized Kohn-Sham Theory for Hybrid Functionals. Physical Review X, 2020, 10, .	8.9	19
26	General Approach for Reducing Continuous Translational Symmetry Errors in Finite Difference Real-Space Calculations. Journal of Chemical Theory and Computation, 2020, 16, 4327-4336.	5.3	1
27	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.	2.8	37
28	Assessment of the Performance of Optimally Tuned Rangeâ€Separated Hybrid Functionals for Nuclear Magnetic Shielding Calculations. Advanced Theory and Simulations, 2020, 3, 2000083.	2.8	7
29	Feâ€porphyrin on Co(001) and Cu(001): A Comparative Dispersionâ€augmented Density Functional Theory Study. Israel Journal of Chemistry, 2020, 60, 870-875.	2.3	0
30	Role of long-range exact exchange in polaron charge transition levels: The case of MgO. Physical Review Materials, 2020, 4, .	2.4	8
31	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.	5.3	8
32	Breakdown of the Static Picture of Defect Energetics in Halide Perovskites: The Case of the Br Vacancy in CsPbBr₃. Journal of Physical Chemistry Letters, 2019, 10, 4490-4498.	4.6	52
33	Spatial Phase Distributions in Solution-Based and Evaporated Csâ€“Pbâ€“Br Thin Films. Journal of Physical Chemistry C, 2019, 123, 17666-17677.	3.1	16
34	Asymptotic behavior of the Hartree-exchange and correlation potentials in ensemble density functional theory. Physical Chemistry Chemical Physics, 2019, 21, 19805-19815.	2.8	14
35	Structure and Morphology of Light-Reflecting Synthetic and Biogenic Polymorphs of Isoxanthopterin: A Comparison. Chemistry of Materials, 2019, 31, 4479-4489.	6.7	12
36	Bulklike band-offset mystery solved through energy minimization: Lessons from perovskite oxide heterojunctions. Physical Review B, 2019, 99, .	3.2	8

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37	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.	2.8	6
38	Mechanically rigid supramolecular assemblies formed from an Fmoc-guanine conjugated peptide nucleic acid. Nature Communications, 2019, 10, 5256.	12.8	24
39	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.	13.7	18
40	Nonmagnetic single-molecule spin-filter based on quantum interference. Nature Communications, 2019, 10, 5565.	12.8	57
41	Constructing the Electronic Structure of CH₃NH₃PbI₃ and CH₃NH₃PbBr₃ Perovskite Thin Films from Single-Crystal Band Structure Measurements. Journal of Physical Chemistry Letters, 2019, 10, 601-609.	4.6	78
42	Comparing time-dependent density functional theory with many-body perturbation theory for semiconductors: Screened range-separated hybrids and the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m plus Bethe-Salpeter approach. Physical Review Materials, 2019, 3, .	2.4	61
43	Transferable screened range-separated hybrids for layered materials: The cases of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></m h-BN. Physical Review Materials, 2019, 3, .	2.4	20
44	Magnetic configurations of open-shell molecules on metals: The case of CuPc and CoPc on silver. Physical Review Materials, 2019, 3, .	2.4	4
45	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.	7.1	39
46	Molecule-Adsorbed Topological Insulator and Metal Surfaces: A Comparative First-Principles Study. Chemistry of Materials, 2018, 30, 1849-1855.	6.7	10
47	Dielectric Screening Meets Optimally Tuned Density Functionals. Advanced Materials, 2018, 30, e1706560.	21.0	108
48	Electronic structure of dipeptides in the gas-phase and as an adsorbed monolayer. Physical Chemistry Chemical Physics, 2018, 20, 6860-6867.	2.8	9
49	Low-lying excited states in crystalline perylene. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 284-289.	7.1	35
50	Effect of Internal Heteroatoms on Level Alignment at Metal/Molecular Monolayer/Si Interfaces. Journal of Physical Chemistry C, 2018, 122, 3312-3325.	3.1	7
51	Charge transfer excitations from exact and approximate ensemble Kohn-Sham theory. Journal of Chemical Physics, 2018, 148, 174101.	3.0	29
52	What Remains Unexplained about the Properties of Halide Perovskites?. Advanced Materials, 2018, 30, e1800691.	21.0	231
53	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.	5.5	23
54	Bioinspired Flexible and Tough Layered Peptide Crystals. Advanced Materials, 2018, 30, 1704551.	21.0	28

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55	Charge Density and Band Offsets at Heterovalent Semiconductor Interfaces. Advanced Theory and Simulations, 2018, 1, 1700001.	2.8	20
56	Vibrational properties of isotopically enriched materials: the case of calcite. RSC Advances, 2018, 8, 33985-33992.	3.6	7
57	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.	5.3	76
58	Photoelectron spectra of copper oxide cluster anions from first principles methods. Journal of Chemical Physics, 2018, 149, 064306.	3.0	8
59	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.	5.3	51
60	Prediction of electronic couplings for molecular charge transfer using optimally tuned range-separated hybrid functionals. Molecular Physics, 2018, 116, 2497-2505.	1.7	15
61	Time-dependent generalized Kohnâ€“Sham theory. European Physical Journal B, 2018, 91, 1.	1.5	75
62	Separation of enantiomers by their enantiospecific interaction with achiral magnetic substrates. Science, 2018, 360, 1331-1334.	12.6	283
63	Terahertz spectroscopy of 2,4,6-trinitrotoluene molecular solids from first principles. Beilstein Journal of Organic Chemistry, 2018, 14, 381-388.	2.2	10
64	Spinâ€€State Energetics of Fe Complexes from an Optimally Tuned Rangeâ€€Separated Hybrid Functional. Chemistry - A European Journal, 2018, 24, 5173-5182.	3.3	38
65	Energy level alignment at molecule-metal interfaces from an optimally tuned range-separated hybrid functional. Journal of Chemical Physics, 2017, 146, .	3.0	59
66	Biologically Controlled Morphology and Twinning in Guanine Crystals. Angewandte Chemie - International Edition, 2017, 56, 9420-9424.	13.8	36
67	Local Polar Fluctuations in Lead Halide Perovskite Crystals. Physical Review Letters, 2017, 118, 136001.	7.8	489
68	Parameter-free driven Liouville-von Neumann approach for time-dependent electronic transport simulations in open quantum systems. Journal of Chemical Physics, 2017, 146, 092331.	3.0	40
69	Light-induced picosecond rotational disordering of the inorganic sublattice in hybrid perovskites. Science Advances, 2017, 3, e1602388.	10.3	149
70	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.	3.1	61
71	Biologically Controlled Morphology and Twinning in Guanine Crystals. Angewandte Chemie, 2017, 129, 9548-9552.	2.0	25
72	Valence electronic structure of cobalt phthalocyanine from an optimally tuned range-separated hybrid functional. Journal of Chemical Physics, 2017, 147, 044301.	3.0	48

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73	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.	4.6	84
74	Valence and Conduction Band Densities of States of Metal Halide Perovskites: A Combined Experimentalâ€“Theoretical Study. Journal of Physical Chemistry Letters, 2016, 7, 2722-2729.	4.6	333
75	Real-space pseudopotential method for computing the vibrational Stark effect. Journal of Chemical Physics, 2016, 145, 174111.	3.0	3
76	Origin and structure of polar domains in doped molecular crystals. Nature Communications, 2016, 7, 13351.	12.8	36
77	Cold denaturation induces inversion of dipole and spin transfer in chiral peptide monolayers. Nature Communications, 2016, 7, 10744.	12.8	83
78	Excited-State Properties of Molecular Solids from First Principles. Annual Review of Physical Chemistry, 2016, 67, 587-616.	10.8	88
79	High Chloride Doping Levels Stabilize the Perovskite Phase of Cesium Lead Iodide. Nano Letters, 2016, 16, 3563-3570.	9.1	247
80	Interlayer Potential for Graphene/h-BN Heterostructures. Journal of Chemical Theory and Computation, 2016, 12, 2896-2905.	5.3	107
81	Optical phonons in methylammonium lead halide perovskites and implications for charge transport. Materials Horizons, 2016, 3, 613-620.	12.2	299
82	Band offset formation at semiconductor heterojunctions through density-based minimization of interface energy. Physical Review B, 2016, 94, .	3.2	17
83	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, 10785-10790.	7.1	77
84	Structural and excited-state properties of oligoacene crystals from first principles. Physical Review B, 2016, 93, .	3.2	89
85	Hybrid organicâ€”inorganic perovskites: low-cost semiconductors with intriguing charge-transport properties. Nature Reviews Materials, 2016, 1, .	48.7	1,173
86	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.	3.1	27
87	Hybrid Organicâ€“Inorganic Perovskites on the Move. Accounts of Chemical Research, 2016, 49, 573-581.	15.6	227
88	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	11
89	Interplay of Bias-Driven Charging and the Vibrational Stark Effect in Molecular Junctions. Nano Letters, 2016, 16, 1104-1109.	9.1	40
90	Enhanced Magnetoresistance in Molecular Junctions by Geometrical Optimization of Spin-Selective Orbital Hybridization. Nano Letters, 2016, 16, 1741-1745.	9.1	35

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91	Theory of Hydrogen Migration in Organicâ€“Inorganic Halide Perovskites. Angewandte Chemie, 2015, 127, 12614-12618.	2.0	8
92	Solid-state optical absorption from optimally tuned time-dependent range-separated hybrid density functional theory. Physical Review B, 2015, 92, .	3.2	210
93	Effect of ensemble generalization on the highest-occupied Kohn-Sham eigenvalue. Journal of Chemical Physics, 2015, 143, 104105.	3.0	16
94	Unusually Large Youngâ€™s Moduli of Amino Acid Molecular Crystals. Angewandte Chemie - International Edition, 2015, 54, 13566-13570.	13.8	83
95	Hybrid Organicâ€“Inorganic Perovskites (HOIPs): Opportunities and Challenges. Advanced Materials, 2015, 27, 5102-5112.	21.0	372
96	Theory of Hydrogen Migration in Organicâ€“Inorganic Halide Perovskites. Angewandte Chemie - International Edition, 2015, 54, 12437-12441.	13.8	134
97	Computational Modelling of Organic Semiconductors: From the Quantum World to Actual Devices. Advanced Functional Materials, 2015, 25, 1913-1914.	14.9	0
98	â€œGuanigmaâ€• The Revised Structure of Biogenic Anhydrous Guanine. Chemistry of Materials, 2015, 27, 8289-8297.	6.7	74
99	Multiscale approach to the electronic structure of doped semiconductor surfaces. Physical Review B, 2015, 91, .	3.2	29
100	Deviations from piecewise linearity in the solid-state limit with approximate density functionals. Journal of Chemical Physics, 2015, 142, 034107.	3.0	42
101	Electronic Transport via Homopeptides: The Role of Side Chains and Secondary Structure. Journal of the American Chemical Society, 2015, 137, 9617-9626.	13.7	101
102	Elimination of the asymptotic fractional dissociation problem in Kohn-Sham density-functional theory using the ensemble-generalization approach. Physical Review A, 2015, 91, .	2.5	26
103	Reliable Energy Level Alignment at Physisorbed Moleculeâ€“Metal Interfaces from Density Functional Theory. Nano Letters, 2015, 15, 2448-2455.	9.1	112
104	Moleculeâ€“Lead Coupling at Molecular Junctions: Relation between the Real- and State-Space Perspectives. Journal of Chemical Theory and Computation, 2015, 11, 4861-4869.	5.3	33
105	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	8
106	Are Mobilities in Hybrid Organicâ€“Inorganic Halide Perovskites Actually â€œHighâ€?. Journal of Physical Chemistry Letters, 2015, 6, 4754-4757.	4.6	197
107	Relating the Physical Structure and Optoelectronic Function of Crystalline TIPSâ€Pentacene. Advanced Functional Materials, 2015, 25, 2038-2046.	14.9	77
108	Structural, Electronic, and Optical Properties of Organic Electronic Materials from Density Functional Theory. , 2015, , .		0

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109	Fundamental gaps with approximate density functionals: The derivative discontinuity revealed from ensemble considerations. Journal of Chemical Physics, 2014, 140, 18A540.	3.0	75
110	Real-space method for highly parallelizable electronic transport calculations. Physical Review B, 2014, 90, .	3.2	10
111	Inter-layer potential for hexagonal boron nitride. Journal of Chemical Physics, 2014, 140, 104106.	3.0	72
112	A self-interaction-free local hybrid functional: Accurate binding energies vis-Ã-vis accurate ionization potentials from Kohn-Sham eigenvalues. Journal of Chemical Physics, 2014, 140, 18A510.	3.0	66
113	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.	5.3	128
114	Infrared Absorption Spectrum of Brushite from First Principles. Chemistry of Materials, 2014, 26, 2934-2942.	6.7	41
115	Gas-Phase Valence-Electron Photoemission Spectroscopy Using Density Functional Theory. Topics in Current Chemistry, 2014, 347, 137-191.	4.0	37
116	One-electron self-interaction and the asymptotics of the Kohnâ€“Sham potential: an impaired relation. Physical Chemistry Chemical Physics, 2014, 16, 14357-14367.	2.8	56
117	State Representation Approach for Atomistic Time-Dependent Transport Calculations in Molecular Junctions. Journal of Chemical Theory and Computation, 2014, 10, 2927-2941.	5.3	56
118	Why Are Diphenylalanine-Based Peptide Nanostructures so Rigid? Insights from First Principles Calculations. Journal of the American Chemical Society, 2014, 136, 963-969.	13.7	136
119	Role of Dispersive Interactions in Determining Structural Properties of Organicâ€“Inorganic Halide Perovskites: Insights from First-Principles Calculations. Journal of Physical Chemistry Letters, 2014, 5, 2728-2733.	4.6	199
120	Experimental and theoretical electronic structure of quinacridone. Physical Review B, 2014, 90, .	3.2	70
121	Simultaneous Determination of Structures, Vibrations, and Frontier Orbital Energies from a Self-Consistent Range-Separated Hybrid Functional. Journal of Physical Chemistry Letters, 2014, 5, 2734-2741.	4.6	49
122	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, 1282-1287.	7.1	63
123	Probing the Orbital Origin of Conductance Oscillations in Atomic Chains. Nano Letters, 2014, 14, 2988-2993.	9.1	22
124	Understanding Molecular Crystals with Dispersion-Inclusive Density Functional Theory: Pairwise Corrections and Beyond. Accounts of Chemical Research, 2014, 47, 3208-3216.	15.6	146
125	Effect of Moleculeâ€“Surface Reaction Mechanism on the Electronic Characteristics and Photovoltaic Performance of Molecularly Modified Si. Journal of Physical Chemistry C, 2013, 117, 22351-22361.	3.1	25
126	Electronic structure of CoPc adsorbed on Ag(100): Evidence for molecule-substrate interaction mediated by Co 3<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>d</mml:mi></mml:math>orbitals. Physical Review B, 2013, 87, .	3.2	54

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127	Gap renormalization of molecular crystals from density-functional theory. Physical Review B, 2013, 88, .	3.2	239
128	Using optimally tuned range separated hybrid functionals in ground-state calculations: Consequences and caveats. Journal of Chemical Physics, 2013, 138, 204115.	3.0	166
129	Locally Refined Multigrid Solution of the All-Electron Kohnâ€“Sham Equation. Journal of Chemical Theory and Computation, 2013, 9, 4744-4760.	5.3	14
130	Effect of Doping Density on the Charge Rearrangement and Interface Dipole at the Moleculeâ€“Silicon Interface. Journal of Physical Chemistry C, 2013, 117, 22422-22427.	3.1	13
131	Atomically Wired Molecular Junctions: Connecting a Single Organic Molecule by Chains of Metal Atoms. Nano Letters, 2013, 13, 1956-1961.	9.1	47
132	Low-Energy Charge-Transfer Excitons in Organic Solids from First-Principles: The Case of Pentacene. Journal of Physical Chemistry Letters, 2013, 4, 2197-2201.	4.6	166
133	Pair-Wise and Many-Body Dispersive Interactions Coupled to an Optimally Tuned Range-Separated Hybrid Functional. Journal of Chemical Theory and Computation, 2013, 9, 3473-3478.	5.3	22
134	Piecewise Linearity of Approximate Density Functionals Revisited: Implications for Frontier Orbital Energies. Physical Review Letters, 2013, 110, 126403.	7.8	110
135	Simulated doping of Si from first principles using pseudoatoms. Physical Review B, 2013, 87, .	3.2	16
136	Charge transport across metal/molecular (alkyl) monolayer-Si junctions is dominated by the LUMO level. Physical Review B, 2012, 85, .	3.2	51
137	Curvature and Frontier Orbital Energies in Density Functional Theory. Journal of Physical Chemistry Letters, 2012, 3, 3740-3744.	4.6	145
138	Hybrids of Organic Molecules and Flat, Oxide-Free Silicon: High-Density Monolayers, Electronic Properties, and Functionalization. Langmuir, 2012, 28, 9920-9929.	3.5	105
139	Dimensionality effects in the electronic structure of organic semiconductors consisting of polar repeat units. Organic Electronics, 2012, 13, 3165-3176.	2.6	19
140	Quasiparticle Spectra from a Nonempirical Optimally Tuned Range-Separated Hybrid Density Functional. Physical Review Letters, 2012, 109, 226405.	7.8	236
141	Quasiparticle and optical spectroscopy of the organic semiconductors pentacene and PTCDA from first principles. Physical Review B, 2012, 85, .	3.2	181
142	Magnetic Properties of Fe/Cu Codoped ZnO Nanocrystals. Journal of Physical Chemistry Letters, 2012, 3, 2009-2014.	4.6	41
143	Excitation Gaps of Finite-Sized Systems from Optimally Tuned Range-Separated Hybrid Functionals. Journal of Chemical Theory and Computation, 2012, 8, 1515-1531.	5.3	765
144	Role of Backbone Charge Rearrangement in the Bond-Dipole and Work Function of Molecular Monolayers. Journal of Physical Chemistry C, 2011, 115, 24888-24892.	3.1	31

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145	Charge-Transfer-Like Ï€â†'Ï€* Excitations in Time-Dependent Density Functional Theory: A Conundrum and Its Solution. Journal of Chemical Theory and Computation, 2011, 7, 2408-2415.	5.3	221
146	Fully Numerical All-Electron Solutions of the Optimized Effective Potential Equation for Diatomic Molecules. Journal of Chemical Theory and Computation, 2011, 7, 2665-2665.	5.3	7
147	Structure and Formation of Synthetic Hemozoin: Insights From First-Principles Calculations. Crystal Growth and Design, 2011, 11, 3332-3341.	3.0	34
148	Electronic level alignment at a metal-molecule interface from a short-range hybrid functional. Journal of Chemical Physics, 2011, 135, 164706.	3.0	71
149	Collectively Induced Quantum-Confined Stark Effect in Monolayers of Molecules Consisting of Polar Repeating Units. Journal of the American Chemical Society, 2011, 133, 18634-18645.	13.7	33
150	Electronic structure of copper phthalocyanine from<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mml:msub><mml:msub><mml:mi>W</mml:mi><mml:r Physical Review B, 2011, 84, .	3.2	86
151	Fundamental and excitation gaps in molecules of relevance for organic photovoltaics from an optimally tuned range-separated hybrid functional. Physical Review B, 2011, 84, .	3.2	281
152	Dispersion Interactions with Density-Functional Theory: Benchmarking Semiempirical and Interatomic Pairwise Corrected Density Functionals. Journal of Chemical Theory and Computation, 2011, 7, 3944-3951.	5.3	265
153	Decoupling Local Disorder and Optical Effects in Infrared Spectra: Differentiating Between Calcites with Different Origins. Advanced Materials, 2011, 23, 550-554.	21.0	91
154	Dissociation of diatomic molecules and the exact-exchange Kohn-Sham potential: The case of LiF. Physical Review A, 2011, 83, .	2.5	37
155	Fundamental Gaps in Finite Systems from Eigenvalues of a Generalized Kohn-Sham Method. Physical Review Letters, 2010, 105, 266802.	7.8	377
156	Polarizability, Susceptibility, and Dielectric Constant of Nanometerâ€Scale Molecular Films: A Microscopic View. Advanced Functional Materials, 2010, 20, 2077-2084.	14.9	53
157	Electronic Properties of Organic-Based Interfaces. MRS Bulletin, 2010, 35, 417-421.	3.5	45
158	Stacking and Registry Effects in Layered Materials: The Case of Hexagonal Boron Nitride. Physical Review Letters, 2010, 105, 046801.	7.8	283
159	Describing Both Dispersion Interactions and Electronic Structure Using Density Functional Theory: The Case of Metalâ^'Phthalocyanine Dimers. Journal of Chemical Theory and Computation, 2010, 6, 81-90.	5.3	109
160	Hg/Molecular Monolayerâ^'Si Junctions: Electrical Interplay between Monolayer Properties and Semiconductor Doping Density. Journal of Physical Chemistry C, 2010, 114, 10270-10279.	3.1	56
161	Examining the role of pseudopotentials in exact-exchange-based Kohn-Sham gaps. Physical Review B, 2009, 80, .	3.2	15
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163	Density functional theory of transition metal phthalocyanines, I:Âelectronic structure of NiPc and CoPcâ€"self-interaction effects. Applied Physics A: Materials Science and Processing, 2009, 95, 159-163.	2.3	105
164	Real-space pseudopotential method for noncollinear magnetism within density functional theory. Solid State Communications, 2009, 149, 177-180.	1.9	8
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