

# Leeor Kronik

## List of Publications by Year in descending order

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249  
papers

22,237  
citations

8732

75  
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9553

142  
g-index

265  
all docs

265  
docs citations

265  
times ranked

19848  
citing authors

#	ARTICLE	IF	CITATIONS
1	Surface photovoltage phenomena: theory, experiment, and applications. <i>Surface Science Reports</i> , 1999, 37, 1-206.	3.8	1,484
2	Hybrid organic–inorganic perovskites: low-cost semiconductors with intriguing charge-transport properties. <i>Nature Reviews Materials</i> , 2016, 1, .	23.3	1,173
3	Orbital-dependent density functionals: Theory and applications. <i>Reviews of Modern Physics</i> , 2008, 80, 3-60.	16.4	1,069
4	Excitation Gaps of Finite-Sized Systems from Optimally Tuned Range-Separated Hybrid Functionals. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1515-1531.	2.3	765
5	Reliable Prediction of Charge Transfer Excitations in Molecular Complexes Using Time-Dependent Density Functional Theory. <i>Journal of the American Chemical Society</i> , 2009, 131, 2818-2820.	6.6	729
6	Local Polar Fluctuations in Lead Halide Perovskite Crystals. <i>Physical Review Letters</i> , 2017, 118, 136001.	2.9	489
7	Fundamental Gaps in Finite Systems from Eigenvalues of a Generalized Kohn-Sham Method. <i>Physical Review Letters</i> , 2010, 105, 266802.	2.9	377
8	Hybrid Organic–Inorganic Perovskites (HOIPs): Opportunities and Challenges. <i>Advanced Materials</i> , 2015, 27, 5102-5112.	11.1	372
9	Valence and Conduction Band Densities of States of Metal Halide Perovskites: A Combined Experimental–Theoretical Study. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 2722-2729.	2.1	333
10	Effects of Sodium on Polycrystalline Cu(In,Ga)Se <sub>2</sub> and Its Solar Cell Performance. <i>Advanced Materials</i> , 1998, 10, 31-36.	11.1	319
11	Prediction of charge-transfer excitations in coumarin-based dyes using a range-separated functional tuned from first principles. <i>Journal of Chemical Physics</i> , 2009, 131, 244119.	1.2	313
12	Surface photovoltage spectroscopy of semiconductor structures: at the crossroads of physics, chemistry and electrical engineering. <i>Surface and Interface Analysis</i> , 2001, 31, 954-965.	0.8	307
13	Optical phonons in methylammonium lead halide perovskites and implications for charge transport. <i>Materials Horizons</i> , 2016, 3, 613-620.	6.4	299
14	PARSEC – the pseudopotential algorithm for real-space electronic structure calculations: recent advances and novel applications to nano-structures. <i>Physica Status Solidi (B): Basic Research</i> , 2006, 243, 1063-1079.	0.7	285
15	Stacking and Registry Effects in Layered Materials: The Case of Hexagonal Boron Nitride. <i>Physical Review Letters</i> , 2010, 105, 046801.	2.9	283
16	Separation of enantiomers by their enantiospecific interaction with achiral magnetic substrates. <i>Science</i> , 2018, 360, 1331-1334.	6.0	283
17	Fundamental and excitation gaps in molecules of relevance for organic photovoltaics from an optimally tuned range-separated hybrid functional. <i>Physical Review B</i> , 2011, 84, .	1.1	281
18	Dispersion Interactions with Density-Functional Theory: Benchmarking Semiempirical and Interatomic Pairwise Corrected Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3944-3951.	2.3	265

#	ARTICLE	IF	CITATIONS
19	High Chloride Doping Levels Stabilize the Perovskite Phase of Cesium Lead Iodide. <i>Nano Letters</i> , 2016, 16, 3563-3570.	4.5	247
20	Gap renormalization of molecular crystals from density-functional theory. <i>Physical Review B</i> , 2013, 88, .	1.1	239
21	Quasiparticle Spectra from a Nonempirical Optimally Tuned Range-Separated Hybrid Density Functional. <i>Physical Review Letters</i> , 2012, 109, 226405.	2.9	236
22	Stability Issues of Cu(In,Ga)Se <sub>2</sub> -Based Solar Cells. <i>Journal of Physical Chemistry B</i> , 2000, 104, 4849-4862.	1.2	235
23	What Remains Unexplained about the Properties of Halide Perovskites?. <i>Advanced Materials</i> , 2018, 30, e1800691.	11.1	231
24	Hybrid Organic-Inorganic Perovskites on the Move. <i>Accounts of Chemical Research</i> , 2016, 49, 573-581.	7.6	227
25	Electrostatic Properties of Ideal and Non-Ideal Polar Organic Monolayers: Implications for Electronic Devices. <i>Advanced Materials</i> , 2007, 19, 4103-4117.	11.1	222
26	Charge-Transfer-Like $\tilde{\epsilon}^*$ Excitations in Time-Dependent Density Functional Theory: A Conundrum and Its Solution. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2408-2415.	2.3	221
27	Electronic structure and spin polarization of Mn <sub>x</sub> Ga <sub>1-x</sub> N. <i>Physical Review B</i> , 2002, 66, .	1.1	214
28	Solid-state optical absorption from optimally tuned time-dependent range-separated hybrid density functional theory. <i>Physical Review B</i> , 2015, 92, .	1.1	210
29	Role of Dispersive Interactions in Determining Structural Properties of Organic-Inorganic Halide Perovskites: Insights from First-Principles Calculations. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2728-2733.	2.1	199
30	Are Mobilities in Hybrid Organic-Inorganic Halide Perovskites Actually "High"? <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 4754-4757.	2.1	197
31	Molecular Control over Semiconductor Surface Electronic Properties: Dicarboxylic Acids on CdTe, CdSe, GaAs, and InP. <i>Journal of the American Chemical Society</i> , 1999, 121, 10545-10553.	6.6	185
32	Quasiparticle and optical spectroscopy of the organic semiconductors pentacene and PTCDA from first principles. <i>Physical Review B</i> , 2012, 85, .	1.1	181
33	Oxygenation and air-annealing effects on the electronic properties of Cu(In,Ga)Se <sub>2</sub> films and devices. <i>Journal of Applied Physics</i> , 1999, 86, 497-505.	1.1	174
34	Using optimally tuned range separated hybrid functionals in ground-state calculations: Consequences and caveats. <i>Journal of Chemical Physics</i> , 2013, 138, 204115.	1.2	166
35	Low-Energy Charge-Transfer Excitons in Organic Solids from First-Principles: The Case of Pentacene. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 2197-2201.	2.1	166
36	Electronic structure of copper phthalocyanine: A comparative density functional theory study. <i>Journal of Chemical Physics</i> , 2008, 128, 164107.	1.2	153

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37	Light-induced picosecond rotational disordering of the inorganic sublattice in hybrid perovskites. <i>Science Advances</i> , 2017, 3, e1602388.	4.7	149
38	Understanding Molecular Crystals with Dispersion-Inclusive Density Functional Theory: Pairwise Corrections and Beyond. <i>Accounts of Chemical Research</i> , 2014, 47, 3208-3216.	7.6	146
39	Curvature and Frontier Orbital Energies in Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3740-3744.	2.1	145
40	Electrical Response of Molecular Chains from Density Functional Theory. <i>Physical Review Letters</i> , 2004, 93, 213002.	2.9	140
41	Yellow luminescence and related deep levels in unintentionally doped GaN films. <i>Physical Review B</i> , 1999, 59, 9748-9751.	1.1	138
42	Why Are Diphenylalanine-Based Peptide Nanostructures so Rigid? Insights from First Principles Calculations. <i>Journal of the American Chemical Society</i> , 2014, 136, 963-969.	6.6	136
43	Theory of Hydrogen Migration in Organic-Inorganic Halide Perovskites. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 12437-12441.	7.2	134
44	Outer-valence Electron Spectra of Prototypical Aromatic Heterocycles from an Optimally Tuned Range-Separated Hybrid Functional. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1934-1952.	2.3	128
45	Hybridization and Bond-Orbital Components in Site-Specific X-Ray Photoelectron Spectra of Rutile TiO <sub>2</sub> . <i>Physical Review Letters</i> , 2002, 89, 077401.	2.9	126
46	Theory of Chirality Induced Spin Selectivity: Progress and Challenges. <i>Advanced Materials</i> , 2022, 34, e2106629.	11.1	119
47	Valence electronic structure of gas-phase 3,4,9,10-perylene tetracarboxylic acid dianhydride: Experiment and theory. <i>Physical Review B</i> , 2006, 73, .	1.1	113
48	Reliable Energy Level Alignment at Physisorbed Molecule-Metal Interfaces from Density Functional Theory. <i>Nano Letters</i> , 2015, 15, 2448-2455.	4.5	112
49	Piecewise Linearity of Approximate Density Functionals Revisited: Implications for Frontier Orbital Energies. <i>Physical Review Letters</i> , 2013, 110, 126403.	2.9	110
50	Describing Both Dispersion Interactions and Electronic Structure Using Density Functional Theory: The Case of Metal-Phthalocyanine Dimers. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 81-90.	2.3	109
51	Dielectric Screening Meets Optimally Tuned Density Functionals. <i>Advanced Materials</i> , 2018, 30, e1706560.	11.1	108
52	Interlayer Potential for Graphene/h-BN Heterostructures. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2896-2905.	2.3	107
53	Density functional theory of transition metal phthalocyanines. I: Electronic structure of NiPc and CoPc self-interaction effects. <i>Applied Physics A: Materials Science and Processing</i> , 2009, 95, 159-163.	1.1	105
54	Hybrids of Organic Molecules and Flat, Oxide-Free Silicon: High-Density Monolayers, Electronic Properties, and Functionalization. <i>Langmuir</i> , 2012, 28, 9920-9929.	1.6	105

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55	Cu(In,Ga)Se <sub>2</sub> Solar Cells: Device Stability Based on Chemical Flexibility. <i>Advanced Materials</i> , 1999, 11, 957-961.	11.1	103
56	Electronic structure of Si(111)-bound alkyl monolayers: Theory and experiment. <i>Physical Review B</i> , 2006, 74, .	1.1	103
57	When to trust photoelectron spectra from Kohn-Sham eigenvalues: The case of organic semiconductors. <i>Physical Review B</i> , 2009, 79, .	1.1	103
58	Electronic Transport via Homopeptides: The Role of Side Chains and Secondary Structure. <i>Journal of the American Chemical Society</i> , 2015, 137, 9617-9626.	6.6	101
59	Density functional theory of transition metal phthalocyanines, II: Electronic structure of MnPc and FePc – symmetry and symmetry breaking. <i>Applied Physics A: Materials Science and Processing</i> , 2009, 95, 165-172.	1.1	100
60	Size-Dependent Spintronic Properties of Dilute Magnetic Semiconductor Nanocrystals. <i>Physical Review Letters</i> , 2005, 94, 236801.	2.9	97
61	Cooperative effects and dipole formation at semiconductor and self-assembled-monolayer interfaces. <i>Physical Review B</i> , 2006, 73, .	1.1	97
62	Interface redox engineering of Cu(In,Ga)Se <sub>2</sub> based solar cells: oxygen, sodium, and chemical bath effects. <i>Thin Solid Films</i> , 2000, 361-362, 353-359.	0.8	96
63	Decoupling Local Disorder and Optical Effects in Infrared Spectra: Differentiating Between Calcites with Different Origins. <i>Advanced Materials</i> , 2011, 23, 550-554.	11.1	91
64	Structural and excited-state properties of oligoacene crystals from first principles. <i>Physical Review B</i> , 2016, 93, .	1.1	89
65	Excited-State Properties of Molecular Solids from First Principles. <i>Annual Review of Physical Chemistry</i> , 2016, 67, 587-616.	4.8	88
66	Electronic structure of copper phthalocyanine from $G_{0W}$ <i>Physical Review B</i> , 2011, 84, .	1.1	86
67	Effect of Solid-State Polarization on Charge-Transfer Excitations and Transport Levels at Organic Interfaces from a Screened Range-Separated Hybrid Functional. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3277-3283.	2.1	84
68	Electronic structure and spin polarization of Mn-containing dilute magnetic III-V semiconductors. <i>Physical Review B</i> , 2001, 64, .	1.1	83
69	Real-space pseudopotential method for computing the electronic properties of periodic systems. <i>Physical Review B</i> , 2004, 69, .	1.1	83
70	Unusually Large Young's Moduli of Amino Acid Molecular Crystals. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 13566-13570.	7.2	83
71	Cold denaturation induces inversion of dipole and spin transfer in chiral peptide monolayers. <i>Nature Communications</i> , 2016, 7, 10744.	5.8	83
72	Surface States and Photovoltaic Effects in CdSe Quantum Dot Films. <i>Journal of the Electrochemical Society</i> , 1998, 145, 1748-1755.	1.3	81

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73	Real-space pseudopotential method for first principles calculations of general periodic and partially periodic systems. <i>Physical Review B</i> , 2008, 78, .	1.1	79
74	Constructing the Electronic Structure of $\text{CH}_3\text{NH}_3\text{PbI}_3$ and $\text{CH}_3\text{NH}_3\text{PbBr}_3$ Perovskite Thin Films from Single-Crystal Band Structure Measurements. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 601-609.	2.1	78
75	Relating the Physical Structure and Optoelectronic Function of Crystalline TIPS-Pentacene. <i>Advanced Functional Materials</i> , 2015, 25, 2038-2046.	7.8	77
76	Tuning electronic transport via hepta-alanine peptides junction by tryptophan doping. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 10785-10790.	3.3	77
77	Local Atomic Order and Infrared Spectra of Biogenic Calcite. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 291-294.	7.2	76
78	Fundamental Gaps of Condensed-Phase Organic Semiconductors from Single-Molecule Calculations using Polarization-Consistent Optimally Tuned Screened Range-Separated Hybrid Functionals. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 6287-6294.	2.3	76
79	Fundamental gaps with approximate density functionals: The derivative discontinuity revealed from ensemble considerations. <i>Journal of Chemical Physics</i> , 2014, 140, 18A540.	1.2	75
80	Time-dependent generalized Kohn-Sham theory. <i>European Physical Journal B</i> , 2018, 91, 1.	0.6	75
81	“Guanigma”: The Revised Structure of Biogenic Anhydrous Guanine. <i>Chemistry of Materials</i> , 2015, 27, 8289-8297.	3.2	74
82	Inter-layer potential for hexagonal boron nitride. <i>Journal of Chemical Physics</i> , 2014, 140, 104106.	1.2	72
83	Optical properties of CdSe quantum dots. <i>Journal of Chemical Physics</i> , 2003, 119, 2284-2287.	1.2	71
84	Electronic level alignment at a metal-molecule interface from a short-range hybrid functional. <i>Journal of Chemical Physics</i> , 2011, 135, 164706.	1.2	71
85	Experimental and theoretical electronic structure of quinacridone. <i>Physical Review B</i> , 2014, 90, .	1.1	70
86	Highest electron affinity as a predictor of cluster anion structures. <i>Nature Materials</i> , 2002, 1, 49-53.	13.3	66
87	A self-interaction-free local hybrid functional: Accurate binding energies vis-à-vis accurate ionization potentials from Kohn-Sham eigenvalues. <i>Journal of Chemical Physics</i> , 2014, 140, 18A510.	1.2	66
88	Voltage tuning of vibrational mode energies in single-molecule junctions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 1282-1287.	3.3	63
89	Time-dependent density-functional calculations for the optical spectra of molecules, clusters, and nanocrystals. <i>Journal of Physics Condensed Matter</i> , 2003, 15, R1517-R1547.	0.7	62
90	Interlayer Potential for Homogeneous Graphene and Hexagonal Boron Nitride Systems: Reparametrization for Many-Body Dispersion Effects. <i>Journal of Physical Chemistry C</i> , 2017, 121, 22826-22835.	1.5	61

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91	Comparing time-dependent density functional theory with many-body perturbation theory for semiconductors: Screened range-separated hybrids and the $G_0W_0$ plus Bethe-Salpeter approach. <i>Physical Review Materials</i> , 2019, 3, .	0.9	61
92	Grain-boundary-controlled transport in GaN layers. <i>Physical Review B</i> , 2000, 61, 15573-15576.	1.1	59
93	Electrostatic Properties of Adsorbed Polar Molecules: Opposite Behavior of a Single Molecule and a Molecular Monolayer. <i>Journal of the American Chemical Society</i> , 2007, 129, 2989-2997.	6.6	59
94	Energy level alignment at molecule-metal interfaces from an optimally tuned range-separated hybrid functional. <i>Journal of Chemical Physics</i> , 2017, 146, .	1.2	59
95	Band diagram of the polycrystalline CdS/Cu(In,Ga)Se <sub>2</sub> heterojunction. <i>Applied Physics Letters</i> , 1995, 67, 1405-1407.	1.5	58
96	Nonmagnetic single-molecule spin-filter based on quantum interference. <i>Nature Communications</i> , 2019, 10, 5565.	5.8	57
97	Ab initio structures and polarizabilities of sodium clusters. <i>Journal of Chemical Physics</i> , 2001, 115, 4322-4332.	1.2	56
98	Hg/Molecular Monolayer/Si Junctions: Electrical Interplay between Monolayer Properties and Semiconductor Doping Density. <i>Journal of Physical Chemistry C</i> , 2010, 114, 10270-10279.	1.5	56
99	One-electron self-interaction and the asymptotics of the Kohn-Sham potential: an impaired relation. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14357-14367.	1.3	56
100	State Representation Approach for Atomistic Time-Dependent Transport Calculations in Molecular Junctions. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2927-2941.	2.3	56
101	Electronic structure of CoPc adsorbed on Ag(100): Evidence for molecule-substrate interaction mediated by Co $d$ orbitals. <i>Physical Review B</i> , 2013, 87, .	1.1	54
102	Ab initio absorption spectra of CdSe clusters. <i>Physical Review B</i> , 2001, 65, .	1.1	53
103	Computing surface dipoles and potentials of self-assembled monolayers from first principles. <i>Applied Surface Science</i> , 2006, 252, 7608-7613.	3.1	53
104	Polarizability, Susceptibility, and Dielectric Constant of Nanometer-Scale Molecular Films: A Microscopic View. <i>Advanced Functional Materials</i> , 2010, 20, 2077-2084.	7.8	53
105	Ab initio calculations for structure and temperature effects on the polarizabilities of Nan( $n < 20$ ) clusters. <i>Physical Review B</i> , 2000, 62, 9992-9995.	1.1	52
106	Breakdown of the Static Picture of Defect Energetics in Halide Perovskites: The Case of the Br Vacancy in CsPbBr <sub>3</sub> . <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4490-4498.	2.1	52
107	Charge transport across metal/molecular (alkyl) monolayer-Si junctions is dominated by the LUMO level. <i>Physical Review B</i> , 2012, 85, .	1.1	51
108	Quantitative Prediction of Optical Absorption in Molecular Solids from an Optimally Tuned Screened Range-Separated Hybrid Functional. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2919-2929.	2.3	51

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109	Long-Range Spin-Selective Transport in Chiral Metal-Organic Crystals with Temperature-Activated Magnetization. <i>ACS Nano</i> , 2020, 14, 16624-16633.	7.3	51
110	Simultaneous Determination of Structures, Vibrations, and Frontier Orbital Energies from a Self-Consistent Range-Separated Hybrid Functional. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2734-2741.	2.1	49
111	Band gaps of crystalline solids from Wannier-localization-based optimal tuning of a screened range-separated hybrid functional. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	49
112	Valence electronic structure of cobalt phthalocyanine from an optimally tuned range-separated hybrid functional. <i>Journal of Chemical Physics</i> , 2017, 147, 044301.	1.2	48
113	Atomically Wired Molecular Junctions: Connecting a Single Organic Molecule by Chains of Metal Atoms. <i>Nano Letters</i> , 2013, 13, 1956-1961.	4.5	47
114	Frontier Orbital Model of Semiconductor Surface Passivation: Dicarboxylic Acids on n- and p-GaAs. <i>Advanced Materials</i> , 2000, 12, 33-37.	11.1	46
115	Electronic Properties of Organic-Based Interfaces. <i>MRS Bulletin</i> , 2010, 35, 417-421.	1.7	45
116	Fully Numerical All-Electron Solutions of the Optimized Effective Potential Equation for Diatomic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1731-1740.	2.3	42
117	Deviations from piecewise linearity in the solid-state limit with approximate density functionals. <i>Journal of Chemical Physics</i> , 2015, 142, 034107.	1.2	42
118	Magnetic Properties of Fe/Cu Codoped ZnO Nanocrystals. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2009-2014.	2.1	41
119	Infrared Absorption Spectrum of Brushite from First Principles. <i>Chemistry of Materials</i> , 2014, 26, 2934-2942.	3.2	41
120	Interplay of Bias-Driven Charging and the Vibrational Stark Effect in Molecular Junctions. <i>Nano Letters</i> , 2016, 16, 1104-1109.	4.5	40
121	Parameter-free driven Liouville-von Neumann approach for time-dependent electronic transport simulations in open quantum systems. <i>Journal of Chemical Physics</i> , 2017, 146, 092331.	1.2	40
122	Distinction between surface and bulk states in surface-photovoltage spectroscopy. <i>Physical Review B</i> , 1994, 50, 1739-1745.	1.1	39
123	Optically functional isoxanthopterin crystals in the mirrored eyes of decapod crustaceans. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 2299-2304.	3.3	39
124	Mechanical and Tribological Properties of Layered Materials under High Pressure: Assessing the Importance of Many-Body Dispersion Effects. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 666-676.	2.3	39
125	Ab initio absorption spectra of Ge nanocrystals. <i>Physical Review B</i> , 2005, 71, .	1.1	38
126	Spin-State Energetics of Fe Complexes from an Optimally Tuned Range-Separated Hybrid Functional. <i>Chemistry - A European Journal</i> , 2018, 24, 5173-5182.	1.7	38



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127	Dissociation of diatomic molecules and the exact-exchange Kohn-Sham potential: The case of LiF. <i>Physical Review A</i> , 2011, 83, .	1.0	37
128	Gas-Phase Valence-Electron Photoemission Spectroscopy Using Density Functional Theory. <i>Topics in Current Chemistry</i> , 2014, 347, 137-191.	4.0	37
129	Piecewise linearity, freedom from self-interaction, and a Coulomb asymptotic potential: three related yet inequivalent properties of the exact density functional. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16467-16481.	1.3	37
130	Band gap determination of semiconductor powders via surface photovoltage spectroscopy. <i>Journal of Applied Physics</i> , 1999, 86, 5573-5577.	1.1	36
131	Parallel implementation of time-dependent density functional theory. <i>Computer Physics Communications</i> , 2003, 156, 22-42.	3.0	36
132	A New "Bottom-Up" Framework for Teaching Chemical Bonding. <i>Journal of Chemical Education</i> , 2008, 85, 1680.	1.1	36
133	Origin and structure of polar domains in doped molecular crystals. <i>Nature Communications</i> , 2016, 7, 13351.	5.8	36
134	Biologically Controlled Morphology and Twinning in Guanine Crystals. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 9420-9424.	7.2	36
135	Cooperative Effects in Molecular Conduction. <i>Journal of Computational and Theoretical Nanoscience</i> , 2008, 5, 535-544.	0.4	36
136	Surface photovoltage spectroscopy of quantum wells and superlattices. <i>Applied Physics Letters</i> , 1996, 68, 879-881.	1.5	35
137	Quantitative assessment of the photosaturation technique. <i>Surface Science</i> , 1998, 409, 485-500.	0.8	35
138	Enhanced Magnetoresistance in Molecular Junctions by Geometrical Optimization of Spin-Selective Orbital Hybridization. <i>Nano Letters</i> , 2016, 16, 1741-1745.	4.5	35
139	Low-lying excited states in crystalline perylene. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 284-289.	3.3	35
140	Radiation Damage to Alkyl Chain Monolayers on Semiconductor Substrates Investigated by Electron Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2006, 110, 21826-21832.	1.2	34
141	Structure and Formation of Synthetic Hemozoin: Insights From First-Principles Calculations. <i>Crystal Growth and Design</i> , 2011, 11, 3332-3341.	1.4	34
142	Collectively Induced Quantum-Confined Stark Effect in Monolayers of Molecules Consisting of Polar Repeating Units. <i>Journal of the American Chemical Society</i> , 2011, 133, 18634-18645.	6.6	33
143	Molecule-lead Coupling at Molecular Junctions: Relation between the Real- and State-Space Perspectives. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4861-4869.	2.3	33
144	Tangential Ligand-Induced Strain in Icosahedral Au <sub>13</sub> . <i>Journal of the American Chemical Society</i> , 2007, 129, 10978-10979.	6.6	32

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145	Laser surface photovoltage spectroscopy: A new tool for the determination of surface state distributions. <i>Applied Physics Letters</i> , 1993, 63, 60-62.	1.5	31
146	Role of Backbone Charge Rearrangement in the Bond-Dipole and Work Function of Molecular Monolayers. <i>Journal of Physical Chemistry C</i> , 2011, 115, 24888-24892.	1.5	31
147	Are Defects in Lead-Halide Perovskites Healed, Tolerated, or Both?. <i>ACS Energy Letters</i> , 2021, 6, 4108-4114.	8.8	31
148	Surface photovoltage spectroscopy of thin films. <i>Journal of Applied Physics</i> , 1996, 79, 8549-8556.	1.1	30
149	Multiscale approach to the electronic structure of doped semiconductor surfaces. <i>Physical Review B</i> , 2015, 91, .	1.1	29
150	Charge transfer excitations from exact and approximate ensemble Kohn-Sham theory. <i>Journal of Chemical Physics</i> , 2018, 148, 174101.	1.2	29
151	The pursuit of stability in halide perovskites: the monovalent cation and the key for surface and bulk self-healing. <i>Materials Horizons</i> , 2021, 8, 1570-1586.	6.4	29
152	Electronic Characterization of Si(100)-Bound Alkyl Monolayers Using Kelvin Probe Force Microscopy. <i>Journal of Physical Chemistry C</i> , 2008, 112, 7145-7150.	1.5	28
153	Bioinspired Flexible and Tough Layered Peptide Crystals. <i>Advanced Materials</i> , 2018, 30, 1704551.	11.1	28
154	Driven Liouville von Neumann Approach for Time-Dependent Electronic Transport Calculations in a Nonorthogonal Basis-Set Representation. <i>Journal of Physical Chemistry C</i> , 2016, 120, 15052-15062.	1.5	27
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