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	Surface photovoltage phenomena: theory, experiment, and applications. Surface Science Reports, 1999, 37, 1-206.	7.2	1,484
2	Hybrid organicâ€"inorganic perovskites: low-cost semiconductors with intriguing charge-transport properties. Nature Reviews Materials, 2016, 1, .	48.7	1,173
3	Orbital-dependent density functionals: Theory and applications. Reviews of Modern Physics, 2008, 80, 3-60.	45.6	1,069
4	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
5	Reliable Prediction of Charge Transfer Excitations in Molecular Complexes Using Time-Dependent Density Functional Theory. Journal of the American Chemical Society, 2009, 131, 2818-2820.	13.7	729
6	Local Polar Fluctuations in Lead Halide Perovskite Crystals. Physical Review Letters, 2017, 118, 136001.	7.8	489
7	Fundamental Gaps in Finite Systems from Eigenvalues of a Generalized Kohn-Sham Method. Physical Review Letters, 2010, 105, 266802.	7.8	377
8	Hybrid Organicâ€"Inorganic Perovskites (HOIPs): Opportunities and Challenges. Advanced Materials, 2015, 27, 5102-5112.	21.0	372
9	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
10	Effects of Sodium on Polycrystalline Cu(In,Ga)Se2 and Its Solar Cell Performance. Advanced Materials, 1998, 10, 31-36.	21.0	319
11	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.	3.0	313
12	Surface photovoltage spectroscopy of semiconductor structures: at the crossroads of physics, chemistry and electrical engineering. Surface and Interface Analysis, 2001, 31, 954-965.	1.8	307
13	Optical phonons in methylammonium lead halide perovskites and implications for charge transport. Materials Horizons, 2016, 3, 613-620.	12.2	299
14	PARSEC â€" the pseudopotential algorithm for real-space electronic structure calculations: recent advances and novel applications to nano-structures. Physica Status Solidi (B): Basic Research, 2006, 243, 1063-1079.	1.5	285
15	Stacking and Registry Effects in Layered Materials: The Case of Hexagonal Boron Nitride. Physical Review Letters, 2010, 105, 046801.	7.8	283
16	Separation of enantiomers by their enantiospecific interaction with achiral magnetic substrates. Science, 2018, 360, 1331-1334.	12.6	283
17	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
18	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

#	Article	IF	Citations
19	High Chloride Doping Levels Stabilize the Perovskite Phase of Cesium Lead Iodide. Nano Letters, 2016, 16, 3563-3570.	9.1	247
20	Gap renormalization of molecular crystals from density-functional theory. Physical Review B, 2013, 88, .	3.2	239
21	Quasiparticle Spectra from a Nonempirical Optimally Tuned Range-Separated Hybrid Density Functional. Physical Review Letters, 2012, 109, 226405.	7.8	236
22	Stability Issues of Cu(In,Ga)Se2-Based Solar Cells. Journal of Physical Chemistry B, 2000, 104, 4849-4862.	2.6	235
23	What Remains Unexplained about the Properties of Halide Perovskites?. Advanced Materials, 2018, 30, e1800691.	21.0	231
24	Hybrid Organicâ€“Inorganic Perovskites on the Move. Accounts of Chemical Research, 2016, 49, 573-581.	15.6	227
25	Electrostatic Properties of Ideal and Nonâ€ideal Polar Organic Monolayers: Implications for Electronic Devices. Advanced Materials, 2007, 19, 4103-4117.	21.0	222
26	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
27	Electronic structure and spin polarization ofMnxGa1â^'xN. Physical Review B, 2002, 66, .	3.2	214
28	Solid-state optical absorption from optimally tuned time-dependent range-separated hybrid density functional theory. Physical Review B, 2015, 92, .	3.2	210
29	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
30	Are Mobilities in Hybrid Organicâ€“Inorganic Halide Perovskites Actually â€œHighâ€?. Journal of Physical Chemistry Letters, 2015, 6, 4754-4757.	4.6	197
31	Molecular Control over Semiconductor Surface Electronic Properties:Â Dicarboxylic Acids on CdTe, CdSe, GaAs, and InP. Journal of the American Chemical Society, 1999, 121, 10545-10553.	13.7	185
32	Quasiparticle and optical spectroscopy of the organic semiconductors pentacene and PTCDA from first principles. Physical Review B, 2012, 85, .	3.2	181
33	Oxygenation and air-annealing effects on the electronic properties of Cu(In,Ga)Se2 films and devices. Journal of Applied Physics, 1999, 86, 497-505.	2.5	174
34	Using optimally tuned range separated hybrid functionals in ground-state calculations: Consequences and caveats. Journal of Chemical Physics, 2013, 138, 204115.	3.0	166
35	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
36	Electronic structure of copper phthalocyanine: A comparative density functional theory study. Journal of Chemical Physics, 2008, 128, 164107.	3.0	153

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37	Light-induced picosecond rotational disordering of the inorganic sublattice in hybrid perovskites. Science Advances, 2017, 3, e1602388.	10.3	149
38	Understanding Molecular Crystals with Dispersion-Inclusive Density Functional Theory: Pairwise Corrections and Beyond. Accounts of Chemical Research, 2014, 47, 3208-3216.	15.6	146
39	Curvature and Frontier Orbital Energies in Density Functional Theory. Journal of Physical Chemistry Letters, 2012, 3, 3740-3744.	4.6	145
40	Electrical Response of Molecular Chains from Density Functional Theory. Physical Review Letters, 2004, 93, 213002.	7.8	140
41	Yellow luminescence and related deep levels in unintentionally doped GaN films. Physical Review B, 1999, 59, 9748-9751.	3.2	138
42	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
43	Theory of Hydrogen Migration in Organicâ€“Inorganic Halide Perovskites. Angewandte Chemie - International Edition, 2015, 54, 12437-12441.	13.8	134
44	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
45	Hybridization and Bond-Orbital Components in Site-Specific X-Ray Photoelectron Spectra of RutileTiO2. Physical Review Letters, 2002, 89, 077401.	7.8	126
46	Theory of Chirality Induced Spin Selectivity: Progress and Challenges. Advanced Materials, 2022, 34, e2106629.	21.0	119
47	Valence electronic structure of gas-phase 3,4,9,10-perylene tetracarboxylic acid dianhydride: Experiment and theory. Physical Review B, 2006, 73, .	3.2	113
48	Reliable Energy Level Alignment at Physisorbed Moleculeâ€“Metal Interfaces from Density Functional Theory. Nano Letters, 2015, 15, 2448-2455.	9.1	112
49	Piecewise Linearity of Approximate Density Functionals Revisited: Implications for Frontier Orbital Energies. Physical Review Letters, 2013, 110, 126403.	7.8	110
50	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
51	Dielectric Screening Meets Optimally Tuned Density Functionals. Advanced Materials, 2018, 30, e1706560.	21.0	108
52	Interlayer Potential for Graphene/h-BN Heterostructures. Journal of Chemical Theory and Computation, 2016, 12, 2896-2905.	5.3	107
53	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
54	Hybrids of Organic Molecules and Flat, Oxide-Free Silicon: High-Density Monolayers, Electronic Properties, and Functionalization. Langmuir, 2012, 28, 9920-9929.	3.5	105

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55	Cu(In,Ga)Se2 Solar Cells: Device Stability Based on Chemical Flexibility. Advanced Materials, 1999, 11, 957-961.	21.0	103
56	Electronic structure of Si(111)-bound alkyl monolayers: Theory and experiment. Physical Review B, 2006, 74, .	3.2	103
57	When to trust photoelectron spectra from Kohn-Sham eigenvalues: The case of organic semiconductors. Physical Review B, 2009, 79, .	3.2	103
58	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
59	Density functional theory of transition metal phthalocyanines, II:Âelectronic structure of MnPc and FePcâ€"symmetry and symmetry breaking. Applied Physics A: Materials Science and Processing, 2009, 95, 165-172.	2.3	100
60	Size-Dependent Spintronic Properties of Dilute Magnetic Semiconductor Nanocrystals. Physical Review Letters, 2005, 94, 236801.	7.8	97
61	Cooperative effects and dipole formation at semiconductor and self-assembled-monolayer interfaces. Physical Review B, 2006, 73, .	3.2	97
62	Interface redox engineering of Cu(In,Ga)Se 2 â€“ based solar cells: oxygen, sodium, and chemical bath effects. Thin Solid Films, 2000, 361-362, 353-359.	1.8	96
63	Decoupling Local Disorder and Optical Effects in Infrared Spectra: Differentiating Between Calcites with Different Origins. Advanced Materials, 2011, 23, 550-554.	21.0	91
64	Structural and excited-state properties of oligoacene crystals from first principles. Physical Review B, 2016, 93, .	3.2	89
65	Excited-State Properties of Molecular Solids from First Principles. Annual Review of Physical Chemistry, 2016, 67, 587-616.	10.8	88
66	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:n Physical Review B, 2011, 84, .	3.2	86
67	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
68	Electronic structure and spin polarization of Mn-containing dilute magnetic III-V semiconductors. Physical Review B, 2001, 64, .	3.2	83
69	Real-space pseudopotential method for computing the electronic properties of periodic systems. Physical Review B, 2004, 69, .	3.2	83
70	Unusually Large Youngâ€™s Moduli of Amino Acid Molecular Crystals. Angewandte Chemie - International Edition, 2015, 54, 13566-13570.	13.8	83
71	Cold denaturation induces inversion of dipole and spin transfer in chiral peptide monolayers. Nature Communications, 2016, 7, 10744.	12.8	83
72	Surface States and Photovoltaic Effects in CdSe Quantum Dot Films. Journal of the Electrochemical Society, 1998, 145, 1748-1755.	2.9	81

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73	Real-space pseudopotential method for first principles calculations of general periodic and partially periodic systems. Physical Review B, 2008, 78, .	3.2	79
74	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
75	Relating the Physical Structure and Optoelectronic Function of Crystalline TIPSâ€Pentacene. Advanced Functional Materials, 2015, 25, 2038-2046.	14.9	77
76	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
77	Local Atomic Order and Infrared Spectra of Biogenic Calcite. Angewandte Chemie - International Edition, 2007, 46, 291-294.	13.8	76
78	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
79	Fundamental gaps with approximate density functionals: The derivative discontinuity revealed from ensemble considerations. Journal of Chemical Physics, 2014, 140, 18A540.	3.0	75
80	Time-dependent generalized Kohnâ€“Sham theory. European Physical Journal B, 2018, 91, 1.	1.5	75
81	â€œGuanigmaâ€• The Revised Structure of Biogenic Anhydrous Guanine. Chemistry of Materials, 2015, 27, 8289-8297.	6.7	74
82	Inter-layer potential for hexagonal boron nitride. Journal of Chemical Physics, 2014, 140, 104106.	3.0	72
83	Optical properties of CdSe quantum dots. Journal of Chemical Physics, 2003, 119, 2284-2287.	3.0	71
84	Electronic level alignment at a metal-molecule interface from a short-range hybrid functional. Journal of Chemical Physics, 2011, 135, 164706.	3.0	71
85	Experimental and theoretical electronic structure of quinacridone. Physical Review B, 2014, 90, .	3.2	70
86	Highest electron affinity as a predictor of cluster anion structures. Nature Materials, 2002, 1, 49-53.	27.5	66
87	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
88	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
89	Time-dependent density-functional calculations for the optical spectra of molecules, clusters, and nanocrystals. Journal of Physics Condensed Matter, 2003, 15, R1517-R1547.	1.8	62
90	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

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91	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
92	Grain-boundary-controlled transport in GaN layers. Physical Review B, 2000, 61, 15573-15576.	3.2	59
93	Electrostatic Properties of Adsorbed Polar Molecules:â€‰ Opposite Behavior of a Single Molecule and a Molecular Monolayer. Journal of the American Chemical Society, 2007, 129, 2989-2997.	13.7	59
94	Energy level alignment at molecule-metal interfaces from an optimally tuned range-separated hybrid functional. Journal of Chemical Physics, 2017, 146, .	3.0	59
95	Band diagram of the polycrystalline CdS/Cu(In,Ga)Se2 heterojunction. Applied Physics Letters, 1995, 67, 1405-1407.	3.3	58
96	Nonmagnetic single-molecule spin-filter based on quantum interference. Nature Communications, 2019, 10, 5565.	12.8	57
97	Ab initiostructures and polarizabilities of sodium clusters. Journal of Chemical Physics, 2001, 115, 4322-4332.	3.0	56
98	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
99	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
100	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
101	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
102	Ab initioabsorption spectra of CdSe clusters. Physical Review B, 2001, 65, .	3.2	53
103	Computing surface dipoles and potentials of self-assembled monolayers from first principles. Applied Surface Science, 2006, 252, 7608-7613.	6.1	53
104	Polarizability, Susceptibility, and Dielectric Constant of Nanometerâ€Scale Molecular Films: A Microscopic View. Advanced Functional Materials, 2010, 20, 2077-2084.	14.9	53
105	Ab initiocalculations for structure and temperature effects on the polarizabilities ofNan(n<~20)clusters. Physical Review B, 2000, 62, 9992-9995.	3.2	52
106	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
107	Charge transport across metal/molecular (alkyl) monolayer-Si junctions is dominated by the LUMO level. Physical Review B, 2012, 85, .	3.2	51
108	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

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109	Long-Range Spin-Selective Transport in Chiral Metalâ€“Organic Crystals with Temperature-Activated Magnetization. ACS Nano, 2020, 14, 16624-16633.	14.6	51
110	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
111	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
112	Valence electronic structure of cobalt phthalocyanine from an optimally tuned range-separated hybrid functional. Journal of Chemical Physics, 2017, 147, 044301.	3.0	48
113	Atomically Wired Molecular Junctions: Connecting a Single Organic Molecule by Chains of Metal Atoms. Nano Letters, 2013, 13, 1956-1961.	9.1	47
114	Frontier Orbital Model of Semiconductor Surface Passivation: Dicarboxylic Acids on n- and p-GaAs. Advanced Materials, 2000, 12, 33-37.	21.0	46
115	Electronic Properties of Organic-Based Interfaces. MRS Bulletin, 2010, 35, 417-421.	3.5	45
116	Fully Numerical All-Electron Solutions of the Optimized Effective Potential Equation for Diatomic Molecules. Journal of Chemical Theory and Computation, 2009, 5, 1731-1740.	5.3	42
117	Deviations from piecewise linearity in the solid-state limit with approximate density functionals. Journal of Chemical Physics, 2015, 142, 034107.	3.0	42
118	Magnetic Properties of Fe/Cu Codoped ZnO Nanocrystals. Journal of Physical Chemistry Letters, 2012, 3, 2009-2014.	4.6	41
119	Infrared Absorption Spectrum of Brushite from First Principles. Chemistry of Materials, 2014, 26, 2934-2942.	6.7	41
120	Interplay of Bias-Driven Charging and the Vibrational Stark Effect in Molecular Junctions. Nano Letters, 2016, 16, 1104-1109.	9.1	40
121	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
122	Distinction between surface and bulk states in surface-photovoltage spectroscopy. Physical Review B, 1994, 50, 1739-1745.	3.2	39
123	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
124	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
125	Ab initioabsorption spectra of Ge nanocrystals. Physical Review B, 2005, 71, .	3.2	38
126	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

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127	Dissociation of diatomic molecules and the exact-exchange Kohn-Sham potential: The case of LiF. Physical Review A, 2011, 83, .	2.5	37
128	Gas-Phase Valence-Electron Photoemission Spectroscopy Using Density Functional Theory. Topics in Current Chemistry, 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. Physical Chemistry Chemical Physics, 2020, 22, 16467-16481.	2.8	37
130	Band gap determination of semiconductor powders via surface photovoltage spectroscopy. Journal of Applied Physics, 1999, 86, 5573-5577.	2.5	36
131	Parallel implementation of time-dependent density functional theory. Computer Physics Communications, 2003, 156, 22-42.	7.5	36
132	A New "Bottom-Up" Framework for Teaching Chemical Bonding. Journal of Chemical Education, 2008, 85, 1680.	2.3	36
133	Origin and structure of polar domains in doped molecular crystals. Nature Communications, 2016, 7, 13351.	12.8	36
134	Biologically Controlled Morphology and Twinning in Guanine Crystals. Angewandte Chemie - International Edition, 2017, 56, 9420-9424.	13.8	36
135	Cooperative Effects in Molecular Conduction. Journal of Computational and Theoretical Nanoscience, 2008, 5, 535-544.	0.4	36
136	Surface photovoltage spectroscopy of quantum wells and superlattices. Applied Physics Letters, 1996, 68, 879-881.	3.3	35
137	Quantitative assessment of the photosaturation technique. Surface Science, 1998, 409, 485-500.	1.9	35
138	Enhanced Magnetoresistance in Molecular Junctions by Geometrical Optimization of Spin-Selective Orbital Hybridization. Nano Letters, 2016, 16, 1741-1745.	9.1	35
139	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
140	Radiation Damage to Alkyl Chain Monolayers on Semiconductor Substrates Investigated by Electron Spectroscopy. Journal of Physical Chemistry B, 2006, 110, 21826-21832.	2.6	34
141	Structure and Formation of Synthetic Hemozoin: Insights From First-Principles Calculations. Crystal Growth and Design, 2011, 11, 3332-3341.	3.0	34
142	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
143	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
144	Tangential Ligand-Induced Strain in Icosahedral Au13. Journal of the American Chemical Society, 2007, 129, 10978-10979.	13.7	32

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145	Laser surface photovoltage spectroscopy: A new tool for the determination of surface state distributions. Applied Physics Letters, 1993, 63, 60-62.	3.3	31
146	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
147	Are Defects in Lead-Halide Perovskites Healed, Tolerated, or Both?. ACS Energy Letters, 2021, 6, 4108-4114.	17.4	31
148	Surface photovoltage spectroscopy of thin films. Journal of Applied Physics, 1996, 79, 8549-8556.	2.5	30
149	Multiscale approach to the electronic structure of doped semiconductor surfaces. Physical Review B, 2015, 91, .	3.2	29
150	Charge transfer excitations from exact and approximate ensemble Kohn-Sham theory. Journal of Chemical Physics, 2018, 148, 174101.	3.0	29
151	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
152	Electronic Characterization of Si(100)-Bound Alkyl Monolayers Using Kelvin Probe Force Microscopy. Journal of Physical Chemistry C, 2008, 112, 7145-7150.	3.1	28
153	Bioinspired Flexible and Tough Layered Peptide Crystals. Advanced Materials, 2018, 30, 1704551.	21.0	28
154	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
155	Quantitative surface photovoltage spectroscopy of semiconductor interfaces. Journal of Electronic Materials, 1995, 24, 379-385.	2.2	26
156	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
157	Yellow luminescence and Fermi level pinning in GaN layers. Applied Physics Letters, 2000, 77, 987.	3.3	25
158	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
159	Biologically Controlled Morphology and Twinning in Guanine Crystals. Angewandte Chemie, 2017, 129, 9548-9552.	2.0	25
160	Effect of air annealing on the electronic properties of CdSCu(In,Ga)Se2 solar cells. Solar Energy Materials and Solar Cells, 1996, 43, 73-78.	6.2	24
161	Mechanically rigid supramolecular assemblies formed from an Fmoc-guanine conjugated peptide nucleic acid. Nature Communications, 2019, 10, 5256.	12.8	24
162	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

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163	Quality control and characterization of Cu(In,Ga)Se2-based thin-film solar cells by surface photovoltage spectroscopy. Solar Energy Materials and Solar Cells, 1998, 51, 21-34.	6.2	22
164	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
165	Probing the Orbital Origin of Conductance Oscillations in Atomic Chains. Nano Letters, 2014, 14, 2988-2993.	9.1	22
166	Surface photovoltage measurements in liquids. Review of Scientific Instruments, 1999, 70, 4032-4036.	1.3	21
167	Photoelectron spectroscopy as a structural probe of intermediate size clusters. Journal of Chemical Physics, 2005, 123, 204312.	3.0	21
168	Electronic characterization of heterojunctions by surface potential monitoring. Journal of Electronic Materials, 1995, 24, 893-901.	2.2	20
169	The Molecularly Controlled Semiconductor Resistor: How does it work?. ACS Applied Materials & Interfaces, 2009, 1, 2679-2683.	8.0	20
170	Charge Density and Band Offsets at Heterovalent Semiconductor Interfaces. Advanced Theory and Simulations, 2018, 1, 1700001.	2.8	20
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