Leeor Kronik

List of Publications by Citations

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	Surface photovoltage phenomena: theory, experiment, and applications. *Surface Science Reports*, **1999**, 37, 1-206	12.9	1337
246	Orbital-dependent density functionals: Theory and applications. *Reviews of Modern Physics*, **2008**, 80, 3-60	40.5	941
245	Hybrid organic□inorganic perovskites: low-cost semiconductors with intriguing charge-transport properties. *Nature Reviews Materials*, **2016**, 1,	73.3	912
244	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
243	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
242	Local Polar Fluctuations in Lead Halide Perovskite Crystals. *Physical Review Letters*, **2017**, 118, 136001	7.4	374
241	Fundamental gaps in finite systems from eigenvalues of a generalized Kohn-Sham method. *Physical Review Letters*, **2010**, 105, 266802	7.4	338
240	Hybrid Organic-Inorganic Perovskites (HOIPs): Opportunities and Challenges. *Advanced Materials*, **2015**, 27, 5102-12	24	325
239	Effects of Sodium on Polycrystalline Cu(In,Ga)Se2 and Its Solar Cell Performance. *Advanced Materials*, **1998**, 10, 31-36	24	282
238	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
237	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
236	Stacking and registry effects in layered materials: the case of hexagonal boron nitride. *Physical Review Letters*, **2010**, 105, 046801	7.4	256
235	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
234	Surface photovoltage spectroscopy of semiconductor structures: at the crossroads of physics, chemistry and electrical engineering. *Surface and Interface Analysis*, **2001**, 31, 954-965	1.5	251
233	PARSEC □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	1.3	242
232	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
231	Optical phonons in methylammonium lead halide perovskites and implications for charge transport. *Materials Horizons*, **2016**, 3, 613-620	14.4	228

230	Electrostatic Properties of Ideal and Non-ideal Polar Organic Monolayers: Implications for Electronic Devices. *Advanced Materials*, **2007**, 19, 4103-4117	24	212
229	High Chloride Doping Levels Stabilize the Perovskite Phase of Cesium Lead Iodide. *Nano Letters*, **2016**, 16, 3563-70	11.5	208
228	Charge-Transfer-Like ππ* 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
227	Stability Issues of Cu(In,Ga)Se2-Based Solar Cells. *Journal of Physical Chemistry B*, **2000**, 104, 4849-4862	3.4	204
226	Quasiparticle spectra from a nonempirical optimally tuned range-separated hybrid density functional. *Physical Review Letters*, **2012**, 109, 226405	7.4	203
225	Electronic structure and spin polarization of MnxGa1−xN. *Physical Review B*, **2002**, 66,	3.3	200
224	Gap renormalization of molecular crystals from density-functional theory. *Physical Review B*, **2013**, 88,	3.3	197
223	Separation of enantiomers by their enantiospecific interaction with achiral magnetic substrates. *Science*, **2018**, 360, 1331-1334	33.3	183
222	Hybrid Organic-Inorganic Perovskites on the Move. *Accounts of Chemical Research*, **2016**, 49, 573-81	24.3	176
221	What Remains Unexplained about the Properties of Halide Perovskites?. *Advanced Materials*, **2018**, 30, e1800691	24	174
220	Solid-state optical absorption from optimally tuned time-dependent range-separated hybrid density functional theory. *Physical Review B*, **2015**, 92,	3.3	171
219	Molecular Control over Semiconductor Surface Electronic Properties: Dicarboxylic Acids on CdTe, CdSe, GaAs, and InP. *Journal of the American Chemical Society*, **1999**, 121, 10545-10553	16.4	169
218	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
217	Are Mobilities in Hybrid Organic-Inorganic Halide Perovskites Actually "High"?. *Journal of Physical Chemistry Letters*, **2015**, 6, 4754-7	6.4	167
216	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	162
215	Quasiparticle and optical spectroscopy of the organic semiconductors pentacene and PTCDA from first principles. *Physical Review B*, **2012**, 85,	3.3	158
214	Electronic structure of copper phthalocyanine: a comparative density functional theory study. *Journal of Chemical Physics*, **2008**, 128, 164107	3.9	143
213	Using optimally tuned range separated hybrid functionals in ground-state calculations: consequences and caveats. *Journal of Chemical Physics*, **2013**, 138, 204115	3.9	140

212	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
211	Curvature and Frontier Orbital Energies in Density Functional Theory. *Journal of Physical Chemistry Letters*, **2012**, 3, 3740-4	6.4	134
210	Electrical response of molecular chains from density functional theory. *Physical Review Letters*, **2004**, 93, 213002	7.4	133
209	Yellow luminescence and related deep levels in unintentionally doped GaN films. *Physical Review B*, **1999**, 59, 9748-9751	3.3	128
208	Understanding molecular crystals with dispersion-inclusive density functional theory: pairwise corrections and beyond. *Accounts of Chemical Research*, **2014**, 47, 3208-16	24.3	121
207	Hybridization and bond-orbital components in site-specific X-ray photoelectron spectra of rutile TiO2. *Physical Review Letters*, **2002**, 89, 077401	7.4	117
206	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
205	Theory of hydrogen migration in organic-inorganic halide perovskites. *Angewandte Chemie - International Edition*, **2015**, 54, 12437-41	16.4	112
204	Valence electronic structure of gas-phase 3,4,9,10-perylene tetracarboxylic acid dianhydride: Experiment and theory. *Physical Review B*, **2006**, 73,	3.3	111
203	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
202	Light-induced picosecond rotational disordering of the inorganic sublattice in hybrid perovskites. *Science Advances*, **2017**, 3, e1602388	14.3	109
201	Electronic structure of Si(111)-bound alkyl monolayers: Theory and experiment. *Physical Review B*, **2006**, 74,	3.3	102
200	Density functional theory of transition metal phthalocyanines, I: electronic structure of NiPc and CoPc□elf-interaction effects. *Applied Physics A: Materials Science and Processing*, **2009**, 95, 159-163	2.6	101
199	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
198	Hybrids of organic molecules and flat, oxide-free silicon: high-density monolayers, electronic properties, and functionalization. *Langmuir*, **2012**, 28, 9920-9	4	98
197	Piecewise linearity of approximate density functionals revisited: implications for frontier orbital energies. *Physical Review Letters*, **2013**, 110, 126403	7.4	97
196	When to trust photoelectron spectra from Kohn-Sham eigenvalues: The case of organic semiconductors. *Physical Review B*, **2009**, 79,	3.3	96
195	Density functional theory of transition metal phthalocyanines, II: electronic structure of MnPc and FePc□ymmetry and symmetry breaking. *Applied Physics A: Materials Science and Processing*, **2009**, 95, 165-172	2.6	95

194	Cooperative effects and dipole formation at semiconductor and self-assembled-monolayer interfaces. *Physical Review B*, **2006**, 73,	3.3	92
193	Size-dependent spintronic properties of dilute magnetic semiconductor nanocrystals. *Physical Review Letters*, **2005**, 94, 236801	7.4	91
192	Cu(In,Ga)Se2 Solar Cells: Device Stability Based on Chemical Flexibility. *Advanced Materials*, **1999**, 11, 957-961	24	89
191	Reliable energy level alignment at physisorbed molecule-metal interfaces from density functional theory. *Nano Letters*, **2015**, 15, 2448-55	11.5	88
190	Interface redox engineering of Cu(In,Ga)Se 2 □based solar cells: oxygen, sodium, and chemical bath effects. *Thin Solid Films*, **2000**, 361-362, 353-359	2.2	87
189	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
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184	Structural and excited-state properties of oligoacene crystals from first principles. *Physical Review B*, **2016**, 93,	3.3	73
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180	Real-space pseudopotential method for first principles calculations of general periodic and partially periodic systems. *Physical Review B*, **2008**, 78,	3.3	66
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171	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
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165	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
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156	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
155	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
154	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
153	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
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137	Ab initio absorption spectra of Ge nanocrystals. *Physical Review B*, **2005**, 71,	3.3	37
136	Deviations from piecewise linearity in the solid-state limit with approximate density functionals. *Journal of Chemical Physics*, **2015**, 142, 034107	3.9	36
135	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
134	Gas-phase valence-electron photoemission spectroscopy using density functional theory. *Topics in Current Chemistry*, **2014**, 347, 137-91		35
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129	Surface photovoltage spectroscopy of quantum wells and superlattices. *Applied Physics Letters*, **1996**, 68, 879-881	3.4	34
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112	Surface photovoltage spectroscopy of thin films. *Journal of Applied Physics*, **1996**, 79, 8549-8556	2.5	27
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110	Biologically Controlled Morphology and Twinning in Guanine Crystals. *Angewandte Chemie - International Edition*, **2017**, 56, 9420-9424	16.4	25
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100	Yellow luminescence and Fermi level pinning in GaN layers. *Applied Physics Letters*, **2000**, 77, 987	3.4	22
99	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	6.4	22
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86	Probing the orbital origin of conductance oscillations in atomic chains. *Nano Letters*, **2014**, 14, 2988-93	11.5	17
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84	Bioinspired Flexible and Tough Layered Peptide Crystals. *Advanced Materials*, **2018**, 30, 1704551	24	17
83	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
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79	Cooperative effects in molecular conduction II: The semiconductor-metal molecular junction. *Journal of Physical Chemistry A*, **2009**, 113, 7451-60	2.8	15
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