Sivan Refaely-Abramson

List of Publications by Year
in descending order

36 papers	3,430 citations	257450 24 h-index	361022 35 g-index

37 all docs	37 docs citations	37 times ranked	3705 citing authors

#	Article	IF	Citations
1	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
2	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
3	Gap renormalization of molecular crystals from density-functional theory. Physical Review B, 2013, 88, .	3.2	239
4	Quasiparticle Spectra from a Nonempirical Optimally Tuned Range-Separated Hybrid Density Functional. Physical Review Letters, 2012, 109, 226405.	7.8	236
5	Solid-state optical absorption from optimally tuned time-dependent range-separated hybrid density functional theory. Physical Review B, 2015, 92, .	3.2	210
6	Identifying substitutional oxygen as a prolific point defect in monolayer transition metal dichalcogenides. Nature Communications, 2019, 10, 3382.	12.8	196
7	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
8	Large Spin-Orbit Splitting of Deep In-Gap Defect States of Engineered Sulfur Vacancies in Monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>WS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></m Physical Review Letters, 2019, 123, 076801.	7.8	120
9	Theory of Chirality Induced Spin Selectivity: Progress and Challenges. Advanced Materials, 2022, 34, e2106629.	21.0	119
10	Defect-Induced Modification of Low-Lying Excitons and Valley Selectivity in Monolayer Transition Metal Dichalcogenides. Physical Review Letters, 2018, 121, 167402.	7.8	109
11	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
12	The role of chalcogen vacancies for atomic defect emission in MoS2. Nature Communications, 2021, 12, 3822.	12.8	94
13	How Substitutional Point Defects in Two-Dimensional WS₂ Induce Charge Localization, Spinâ€“Orbit Splitting, and Strain. ACS Nano, 2019, 13, 10520-10534.	14.6	86
14	Cold denaturation induces inversion of dipole and spin transfer in chiral peptide monolayers. Nature Communications, 2016, 7, 10744.	12.8	83
15	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
16	Experimental and theoretical electronic structure of quinacridone. Physical Review B, 2014, 90, .	3.2	70
17	Long-Lived Correlated Triplet Pairs in a Ï€-Stacked Crystalline Pentacene Derivative. Journal of the American Chemical Society, 2018, 140, 2326-2335.	13.7	68
18	Energy level alignment at molecule-metal interfaces from an optimally tuned range-separated hybrid functional. Journal of Chemical Physics, 2017, 146, .	3.0	59

#	Article	IF	Citations
19	Origins of Singlet Fission in Solid Pentacene from an abÂinitio Greenâ€™s Function Approach. Physical Review Letters, 2017, 119, 267401.	7.8	55
20	Rational Passivation of Sulfur Vacancy Defects in Two-Dimensional Transition Metal Dichalcogenides. ACS Nano, 2021, 15, 8780-8789.	14.6	52
21	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
22	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
23	Optical absorption of interlayer excitons in transition-metal dichalcogenide heterostructures. Science, 2022, 376, 406-410.	12.6	42
24	Probing Charge Transport through Peptide Bonds. Journal of Physical Chemistry Letters, 2018, 9, 763-767.	4.6	38
25	Quantum Phase Transitions of Trilayer Excitons in Atomically Thin Heterostructures. Physical Review Letters, 2020, 125, 255301.	7.8	21
26	Signatures of Dimensionality and Symmetry in Exciton Band Structure: Consequences for Exciton Dynamics and Transport. Nano Letters, 2021, 21, 7644-7650.	9.1	21
27	Anisotropic 2D excitons unveiled in organicâ€“inorganic quantum wells. Materials Horizons, 2021, 8, 197-208.	12.2	17
28	First-Principles Approach to the Conductance of Covalently Bound Molecular Junctions. Journal of Physical Chemistry C, 2019, 123, 6379-6387.	3.1	10
29	Electronic structure of dipeptides in the gas-phase and as an adsorbed monolayer. Physical Chemistry Chemical Physics, 2018, 20, 6860-6867.	2.8	9
30	Bright excitonic multiplexing mediated by dark exciton transition in two-dimensional TMDCs at room temperature. Materials Horizons, 2022, 9, 1089-1098.	12.2	8
31	Mixed excitonic nature in water-oxidized <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BiVO</mml:mi><mml:mn>4</mml:mn></mml:msub></mml surfaces with defects. Physical Review Materials, 2022, 6, .	2.4	5
32	Layer-Dependent Quasiparticle Electronic Structure of the P3HT:PCBM Interface from a First-Principles Substrate Screening GW Approach. Journal of Physical Chemistry C, 2020, 124, 13592-13601.	3.1	4
33	Identifying Hidden Intracell Symmetries in Molecular Crystals and Their Impact for Multiexciton Generation. Journal of Physical Chemistry Letters, 2022, 13, 747-753.	4.6	3
34	Exciton Modulation in Perylene-Based Molecular Crystals Upon Formation of a Metal-Organic Interface From Many-Body Perturbation Theory. Frontiers in Chemistry, 2021, 9, 743391.	3.6	2
35	From exciton dispersion to exciton dynamics in functional materials. , 0, , .		0
36	Excited-State Properties of Perylene-Based Organic-Inorganic Interfaces from First Principles. , 0, , .		0