Sahar Sharifzadeh

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/9199523/publications.pdf

Version: 2024-02-01

45 papers	2,347 citations	377584 21 h-index	299063 42 g-index
46 all docs	46 docs citations	46 times ranked	3215 citing authors

#	Article	IF	Citations
1	Vibronic Photoexcitation Dynamics of Perylene Diimide: Computational Insights. Journal of Physical Chemistry A, 2022, 126, 733-741.	1.1	1
2	Electronic Raman scattering in the 2D antiferromagnet NiPS ₃. Science Advances, 2022, 8, eabl7707.	4.7	13
3	Electronic Structure of de Novo Peptide ACC-Hex from First Principles. Journal of Physical Chemistry B, 2022, 126, 4289-4298.	1.2	2
4	Tuning spinâ€“orbit coupling in (6,5) single-walled carbon nanotube doped with sp3 defects. Journal of Applied Physics, 2021, 129, .	1.1	6
5	Excitonâ€“Phonon Interactions in Monolayer Germanium Selenide from First Principles. Journal of Physical Chemistry Letters, 2021, 12, 3802-3808.	2.1	9
6	Spin-induced linear polarization of photoluminescence in antiferromagnetic van der Waals crystals. Nature Materials, 2021, 20, 964-970.	13.3	59
7	Modeling Excited States of Point Defects in Materials from Many-Body Perturbation Theory. , 2021, 3, 862-874.		3
8	Atomic understanding of structural deformations upon ablation of graphene. Nano Select, 2021, 2, 2215-2224.	1.9	2
9	Vibrational Signature of Metallophilic Interactions in [Pt(terpy)Cl][Au(CN)₂]. Journal of Physical Chemistry C, 2021, 125, 22188-22194.	1.5	7
10	sp³-Functionalization of Single-Walled Carbon Nanotubes Creates Localized Spins. ACS Nano, 2020, 14, 17675-17682.	7.3	17
11	Microscopic Theory of Plasmons in Substrate-Supported Borophene. Nano Letters, 2020, 20, 2986-2992.	4.5	11
12	Accurate First-Principles Calculation of the Vibronic Spectrum of Stacked Perylene Tetracarboxylic Acid Diimides. Journal of Physical Chemistry A, 2020, 124, 3055-3063.	1.1	16
13	Photoexcitation dynamics in perylene diimide dimers. Journal of Chemical Physics, 2020, 153, 244117.	1.2	8
14	Tuned and screened range-separated hybrid density functional theory for describing electronic and optical properties of defective gallium nitride. Physical Review Materials, 2020, 4, .	0.9	17
15	Localized excitons in defective monolayer germanium selenide. Physical Review Materials, 2020, 4, .	0.9	4
16	Molecular dynamics simulations of DNA-inspired macromolecules from perylenediimide base surrogates. Synthetic Metals, 2019, 253, 146-152.	2.1	6
17	Assessing the Role of Intermolecular Interactions in a Perylene-Based Nanowire Using First-Principles Many-Body Perturbation Theory. Journal of Physical Chemistry Letters, 2019, 10, 2842-2848.	2.1	6
18	Defect-induced exciton localization in bulk gallium nitride from many-body perturbation theory. Physical Review Materials, 2019, 3, .	0.9	11

#	Article	IF	Citations
19	Many-body perturbation theory for understanding optical excitations in organic molecules and solids. Journal of Physics Condensed Matter, 2018, 30, 153002.	0.7	30
20	First-Principles Investigation of Borophene as a Monolayer Transparent Conductor. Journal of Physical Chemistry C, 2018, 122, 4037-4045.	1.5	89
21	Low-lying excited states in crystalline perylene. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 284-289.	3.3	35
22	The elastic constants of rubrene determined by Brillouin scattering and density functional theory. Applied Physics Letters, 2017, 110, .	1.5	15
23	Unexpected length dependence of excited-state charge transfer dynamics for surface-confined perylenediimide ensembles. Materials Horizons, 2017, 4, 437-441.	6.4	5
24	Fine-Tuning the Optoelectronic Properties of Freestanding Borophene by Strain. ACS Omega, 2017, 2, 8290-8299.	1.6	46
25	Lengthâ€Independent Charge Transport in Chimeric Molecular Wires. Angewandte Chemie, 2016, 128, 14479-14483.	1.6	1
26	Lengthâ€Independent Charge Transport in Chimeric Molecular Wires. Angewandte Chemie - International Edition, 2016, 55, 14267-14271.	7.2	13
27	Structural and excited-state properties of oligoacene crystals from first principles. Physical Review B, 2016, 93, .	1.1	89
28	Solid-state optical absorption from optimally tuned time-dependent range-separated hybrid density functional theory. Physical Review B, 2015, 92, .	1.1	210
29	Numerical integration for ab initio many-electron self energy calculations within the GW approximation. Journal of Computational Physics, 2015, 286, 1-13.	1.9	15
30	Low-Lying Electronic Excited States of Pentacene Oligomers: A Comparative Electronic Structure Study in the Context of Singlet Fission. Journal of Chemical Theory and Computation, 2015, 11, 147-156.	2.3	63
31	GW100: Benchmarking G₀W₀ for Molecular Systems. Journal of Chemical Theory and Computation, 2015, 11, 5665-5687.	2.3	280
32	Relating the Physical Structure and Optoelectronic Function of Crystalline TIPSâ€Pentacene. Advanced Functional Materials, 2015, 25, 2038-2046.	7.8	77
33	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.	2.3	128
34	Effects of self-consistency and plasmon-pole models on<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 for closed-shell molecules. Physical Review B, 2014, 90, .	1.1	24
35	Gap renormalization of molecular crystals from density-functional theory. Physical Review B, 2013, 88, .	1.1	239
36	Low-Energy Charge-Transfer Excitons in Organic Solids from First-Principles: The Case of Pentacene. Journal of Physical Chemistry Letters, 2013, 4, 2197-2201.	2.1	166

#	Article	IF	Citations
37	Quasiparticle Spectra from a Nonempirical Optimally Tuned Range-Separated Hybrid Density Functional. Physical Review Letters, 2012, 109, 226405.	2.9	236
38	Quasiparticle and optical spectroscopy of the organic semiconductors pentacene and PTCDA from first principles. Physical Review B, 2012, 85, .	1.1	181
39	Quantum mechanical modeling of electronic excitations in metal oxides: Magnesia as a prototype. Chemical Physics Letters, 2012, 519-520, 18-24.	1.2	29
40	Relating Trends in First-Principles Electronic Structure and Open-Circuit Voltage in Organic Photovoltaics. Journal of Physical Chemistry Letters, 2011, 2, 2531-2537.	2.1	45
41	Origin of tunneling lineshape trends for Kondo states of Co adatoms on coinage metal surfaces. Journal of Physics Condensed Matter, 2009, 21, 355501.	0.7	9
42	All-electron embedded correlated wavefunction theory for condensed matter electronic structure. Chemical Physics Letters, 2009, 470, 347-352.	1.2	40
43	Embedded Configuration Interaction Description of CO on Cu(111):â€‰ Resolution of the Site Preference Conundrum. Journal of Physical Chemistry C, 2008, 112, 4649-4657.	1.5	47
44	Errata to â€œA Microfabricated Electrochemical Oxygen Generator for High-Density Cell Culture Arraysâ€• Journal of Microelectromechanical Systems, 2004, 13, 386-386.	1.7	0
45	A microfabricated electrochemical oxygen generator for high-density cell culture arrays. Journal of Microelectromechanical Systems, 2003, 12, 590-599.	1.7	37