Noa Marom

List of Publications by Year
in descending order

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Version: 2024-02-01

59 papers	3,272 citations	201575 27 h-index	143943 57 g-index
61 all docs	61 docs citations	61 times ranked	3808 citing authors

#	Article	IF	Citations
1	Electronic Structure of InAs and InSb Surfaces: Density Functional Theory and Angleâ€Resolved Photoemission Spectroscopy. Advanced Quantum Technologies, 2022, 5, .	1.8	6
2	Best practices for first-principles simulations of epitaxial inorganic interfaces. Journal of Physics Condensed Matter, 2022, 34, 233002.	0.7	6
3	An energetics assessment of benzo[a]tetracene and benzo[a]pyrene as tripletâ€“triplet annihilation emitters. Molecular Systems Design and Engineering, 2022, 7, 889-898.	1.7	2
4	Finding predictive models for singlet fission by machine learning. Npj Computational Materials, 2022, 8, .	3.5	4
5	Performance of Dispersion-Inclusive Density Functional Theory Methods for Energetic Materials. Journal of Chemical Theory and Computation, 2022, 18, 4456-4471.	2.3	6
6	Crystal structure prediction of energetic materials and a twisted arene with Genarris and GAtor. CrystEngComm, 2021, 23, 6023-6038.	1.3	15
7	Dependence of the electronic structure of the EuS/InAs interface on the bonding configuration. Physical Review Materials, 2021, 5, .	0.9	10
8	3D Electron Diffraction Structure Determination of Terrylene, a Promising Candidate for Intermolecular Singlet Fission. ChemPhysChem, 2021, 22, 1631-1637.	1.0	10
9	Structure prediction of epitaxial inorganic interfaces by lattice and surface matching with Ogre. Journal of Chemical Physics, 2021, 155, 034111.	1.2	7
10	First-principles feasibility assessment of a topological insulator at the InAs/GaSb interface. Physical Review Materials, 2021, 5, .	0.9	9
11	Assessing Zethrene Derivatives as Singlet Fission Candidates Based on Multiple Descriptors. Journal of Physical Chemistry C, 2020, 124, 26134-26143.	1.5	10
12	Machine Learned Model for Solid Form Volume Estimation Based on Packing-Accessible Surface and Molecular Topological Fragments. Journal of Physical Chemistry A, 2020, 124, 10330-10345.	1.1	9
13	Machine learning the Hubbard U parameter in DFT+U using Bayesian optimization. Npj Computational Materials, 2020, 6, .	3.5	80
14	An energetics perspective on why there are so few tripletâ€“triplet annihilation emitters. Journal of Materials Chemistry C, 2020, 8, 10816-10824.	2.7	32
15	Ogre: A Python package for molecular crystal surface generation with applications to surface energy and crystal habit prediction. Journal of Chemical Physics, 2020, 152, 244122.	1.2	15
16	Pyrene-stabilized acenes as intermolecular singlet fission candidates: Importance of exciton wave-function convergence. Journal of Physics Condensed Matter, 2020, 32, 184001.	0.7	15
17	Genarris 2.0: A random structure generator for molecular crystals. Computer Physics Communications, 2020, 250, 107170.	3.0	15
18	Topological properties of SnSe/EuS and SnTe/CaTe interfaces. Physical Review Materials, 2020, 4, .	0.9	11

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19	Anomalous pressure dependence of the electronic properties of molecular crystals explained by changes in intermolecular electronic coupling. Synthetic Metals, 2019, 253, 9-19.	2.1	4
20	Phenylated Acene Derivatives as Candidates for Intermolecular Singlet Fission. Journal of Physical Chemistry C, 2019, 123, 5890-5899.	1.5	20
21	GAtor: A First-Principles Genetic Algorithm for Molecular Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2018, 14, 2246-2264.	2.3	86
22	Evolutionary niching in the GAtor genetic algorithm for molecular crystal structure prediction. Faraday Discussions, 2018, 211, 61-77.	1.6	13
23	Genarris: Random generation of molecular crystal structures and fast screening with a Harris approximation. Journal of Chemical Physics, 2018, 148, 241701.	1.2	21
24	High-Throughput Pressure-Dependent Density Functional Theory Investigation of Herringbone Polycyclic Aromatic Hydrocarbons: Part 2. Pressure-Dependent Electronic Properties. Journal of Physical Chemistry C, 2018, 122, 23828-23844.	1.5	11
25	High-Throughput Pressure-Dependent Density Functional Theory Investigation of Herringbone Polycyclic Aromatic Hydrocarbons: Part 1. Pressure-Dependent Structure Trends. Journal of Physical Chemistry C, 2018, 122, 23815-23827.	1.5	9
26	Structure searching methods: general discussion. Faraday Discussions, 2018, 211, 133-180.	1.6	3
27	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. Faraday Discussions, 2018, 211, 325-381.	1.6	7
28	On the possibility of singlet fission in crystalline quaterrylene. Journal of Chemical Physics, 2018, 148, 184101.	1.2	21
29	Accurate description of the electronic structure of organic semiconductors byGWmethods. Journal of Physics Condensed Matter, 2017, 29, 103003.	0.7	26
30	Accurate Valence Ionization Energies from Kohnâ€“Sham Eigenvalues with the Help of Potential Adjustors. Journal of Chemical Theory and Computation, 2017, 13, 4726-4740.	2.3	11
31	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	0.5	445
32	Effect of packing motifs on the energy ranking and electronic properties of putative crystal structures of tricyano-1,4-dithiino[c]-isothiazole. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 562-570.	0.5	17
33	Effect of crystal packing on the excitonic properties of rubrene polymorphs. CrystEngComm, 2016, 18, 7353-7362.	1.3	57
34	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules I. Reference Data at the CCSD(T) Complete Basis Set Limit. Journal of Chemical Theory and Computation, 2016, 12, 595-604.	2.3	69
35	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules IV: Electron-Propagator Methods. Journal of Chemical Theory and Computation, 2016, 12, 627-637.	2.3	56
36	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules II: Non-Empirically Tuned Long-Range Corrected Hybrid Functionals. Journal of Chemical Theory and Computation, 2016, 12, 605-614.	2.3	78

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37	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules III: A Benchmark of GW Methods. Journal of Chemical Theory and Computation, 2016, 12, 615-626.	2.3	154
38	Computational design of nanoclusters by property-based genetic algorithms: Tuning the electronic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>(</mml:mo><mml:msub><mml:mi>TiO</mml:mi><mml:mi><mml:n Physical Review B, 2015, 91, .	1.1	29
39	Beyond 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></mm A second-order screened exchange correction. Physical Review B, 2015, 92, .	1.1	49
40	A first-principles study of the electronic and structural properties of Sb and F doped SnO2 nanocrystals. Journal of Chemical Physics, 2015, 142, 044704.	1.2	9
41	Real space pseudopotential calculations for size trends in Ga- and Al-doped zinc oxide nanocrystals with wurtzite and zincblende structures. Journal of Chemical Physics, 2014, 141, 094309.	1.2	7
42	Size Effects in the Interface Level Alignment of Dye-Sensitized TiO₂ Clusters. Journal of Physical Chemistry Letters, 2014, 5, 2395-2401.	2.1	28
43	The Malaria Pigment Hemozoin Comprises at Most Four Different Isomer Units in Two Crystalline Models: Chiral as Based on a Biochemical Hypothesis or Centrosymmetric Made of Enantiomorphous Sectors. Crystal Growth and Design, 2014, 14, 1543-1554.	1.4	11
44	Electrodynamic response and stability of molecular crystals. Physical Review B, 2013, 87, .	1.1	40
45	Manyâ€Body Dispersion Interactions in Molecular Crystal Polymorphism. Angewandte Chemie - International Edition, 2013, 52, 6629-6632.	7.2	149
46	Strategy for finding a reliable starting point for<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> for molecules. Physical Review B, 2012, 86, .	1.1	106
47	Assessment of the performance of tuned range-separated hybrid density functionals in predicting accurate quasiparticle spectra. Physical Review B, 2012, 86, .	1.1	58
48	Structure Selection Based on High Vertical Electron Affinity for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>Clusters. Physical Review Letters, 2012, 108, 106801.	2.9	52
49	Benchmark of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>methods for azabenzenes. Physical Review B, 2012, 86, .	1.1	154
50	Theoretical Design of a Shallow Donor in Diamond by Lithium-Nitrogen Codoping. Physical Review Letters, 2012, 108, 226404.	2.9	20
51	Structure and Formation of Synthetic Hemozoin: Insights From First-Principles Calculations. Crystal Growth and Design, 2011, 11, 3332-3341.	1.4	34
52	Electronic structure of dye-sensitized TiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>clusters from many-body perturbation theory. Physical Review B, 2011, 84, .	1.1	41
53	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> Physical Review B, 2011, 84, .	1.1	86
54	Dispersion Interactions with Density-Functional Theory: Benchmarking Semiempirical and Interatomic Pairwise Corrected Density Functionals. Journal of Chemical Theory and Computation, 2011, 7, 3944-3951.	2.3	265

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55	Stacking and Registry Effects in Layered Materials: The Case of Hexagonal Boron Nitride. Physical Review Letters, 2010, 105, 046801.	2.9	283
56	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.	2.3	109
57	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.	1.1	100
58	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.	1.1	105
59	Electronic structure of copper phthalocyanine: A comparative density functional theory study. Journal of Chemical Physics, 2008, 128, 164107.	1.2	153