

# 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	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
2	Stacking and Registry Effects in Layered Materials: The Case of Hexagonal Boron Nitride. Physical Review Letters, 2010, 105, 046801.	2.9	283
3	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
4	Benchmark of $\langle G \rangle_W$ methods for azabenzenes. Physical Review B, 2012, 86, .	1.1	154
5	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules III: A Benchmark of $\langle CW \rangle$ Methods. Journal of Chemical Theory and Computation, 2016, 12, 615-626.	2.3	154
6	Electronic structure of copper phthalocyanine: A comparative density functional theory study. Journal of Chemical Physics, 2008, 128, 164107.	1.2	153
7	Many-Body Dispersion Interactions in Molecular Crystal Polymorphism. Angewandte Chemie - International Edition, 2013, 52, 6629-6632.	7.2	149
8	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.	2.3	109
9	Strategy for finding a reliable starting point for $\langle G \rangle_{W_0}$ for molecules. Physical Review B, 2012, 86, .	1.1	106
10	Density functional theory of transition metal phthalocyanines, I: Electronic structure of NiPc and CoPc self-interaction effects. Applied Physics A: Materials Science and Processing, 2009, 95, 159-163.	1.1	105
11	Density functional theory of transition metal phthalocyanines, II: Electronic structure of MnPc and FePc symmetry and symmetry breaking. Applied Physics A: Materials Science and Processing, 2009, 95, 165-172.	1.1	100
12	Electronic structure of copper phthalocyanine from $\langle G \rangle_{W_0}$ Physical Review B, 2011, 84, .	1.1	86
13	GATOR: A First-Principles Genetic Algorithm for Molecular Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2018, 14, 2246-2264.	2.3	86
14	Machine learning the Hubbard U parameter in DFT+U using Bayesian optimization. Npj Computational Materials, 2020, 6, .	3.5	80
15	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
16	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
17	Assessment of the performance of tuned range-separated hybrid density functionals in predicting accurate quasiparticle spectra. Physical Review B, 2012, 86, .	1.1	58
18	Effect of crystal packing on the excitonic properties of rubrene polymorphs. CrystEngComm, 2016, 18, 7353-7362.	1.3	57

#	ARTICLE	IF	CITATIONS
19	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules IV: Electron-Propagator Methods. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 627-637.	2.3	56
20	Structure Selection Based on High Vertical Electron Affinity for $\text{TiO}_2$ Clusters. <i>Physical Review Letters</i> , 2012, 108, 106801.	2.9	52
21	Beyond the $\text{GW}$ approximation: A second-order screened exchange correction. <i>Physical Review B</i> , 2015, 92, .	1.1	41
22	Electronic structure of dye-sensitized $\text{TiO}_2$ clusters from many-body perturbation theory. <i>Physical Review B</i> , 2011, 84, .	1.1	40
23	Electrodynamic response and stability of molecular crystals. <i>Physical Review B</i> , 2013, 87, .	1.4	34
24	Structure and Formation of Synthetic Hemozoin: Insights From First-Principles Calculations. <i>Crystal Growth and Design</i> , 2011, 11, 3332-3341.	2.7	32
25	An energetics perspective on why there are so few triplet-triplet annihilation emitters. <i>Journal of Materials Chemistry C</i> , 2020, 8, 10816-10824.	1.1	29
26	Computational design of nanoclusters by property-based genetic algorithms: Tuning the electronic properties of $\text{TiO}_2$ clusters. <i>Physical Review B</i> , 2015, 91, .	2.1	28
27	Size Effects in the Interface Level Alignment of Dye-Sensitized $\text{TiO}_2$ Clusters. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2395-2401.	0.7	26
28	Accurate description of the electronic structure of organic semiconductors by $\text{GW}$ methods. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 103003.	1.2	21
29	Genarris: Random generation of molecular crystal structures and fast screening with a Harris approximation. <i>Journal of Chemical Physics</i> , 2018, 148, 241701.	1.2	21
30	On the possibility of singlet fission in crystalline quaterrylene. <i>Journal of Chemical Physics</i> , 2018, 148, 184101.	2.9	20
31	Theoretical Design of a Shallow Donor in Diamond by Lithium-Nitrogen Codoping. <i>Physical Review Letters</i> , 2012, 108, 226404.	1.5	20
32	Phenylated Acene Derivatives as Candidates for Intermolecular Singlet Fission. <i>Journal of Physical Chemistry C</i> , 2019, 123, 5890-5899.	0.5	17
33	Effect of packing motifs on the energy ranking and electronic properties of putative crystal structures of tricyano-1,4-dithiino[ <i>c</i> ]-isothiazole. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 562-570.	1.2	15
34	Ogre: A Python package for molecular crystal surface generation with applications to surface energy and crystal habit prediction. <i>Journal of Chemical Physics</i> , 2020, 152, 244122.	0.7	15
35	Pyrene-stabilized acenes as intermolecular singlet fission candidates: Importance of exciton wave-function convergence. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 184001.	3.0	15
36	Genarris 2.0: A random structure generator for molecular crystals. <i>Computer Physics Communications</i> , 2020, 250, 107170.		

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37	Crystal structure prediction of energetic materials and a twisted arene with Genarris and GAtor. CrystEngComm, 2021, 23, 6023-6038.	1.3	15
38	Evolutionary niching in the GAtor genetic algorithm for molecular crystal structure prediction. Faraday Discussions, 2018, 211, 61-77.	1.6	13
39	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
40	Accurate Valence Ionization Energies from Kohn-Sham Eigenvalues with the Help of Potential Adjustors. Journal of Chemical Theory and Computation, 2017, 13, 4726-4740.	2.3	11
41	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
42	Topological properties of SnSe/EuS and SnTe/CaTe interfaces. Physical Review Materials, 2020, 4, .	0.9	11
43	Assessing Zethrene Derivatives as Singlet Fission Candidates Based on Multiple Descriptors. Journal of Physical Chemistry C, 2020, 124, 26134-26143.	1.5	10
44	Dependence of the electronic structure of the EuS/InAs interface on the bonding configuration. Physical Review Materials, 2021, 5, .	0.9	10
45	3D Electron Diffraction Structure Determination of Terrylene, a Promising Candidate for Intermolecular Singlet Fission. ChemPhysChem, 2021, 22, 1631-1637.	1.0	10
46	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
47	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
48	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
49	First-principles feasibility assessment of a topological insulator at the InAs/GaSb interface. Physical Review Materials, 2021, 5, .	0.9	9
50	Real space pseudopotential calculations for size trends in Ga- and Al-doped zinc oxide nanocrystals with wurtzite and zinblende structures. Journal of Chemical Physics, 2014, 141, 094309.	1.2	7
51	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. Faraday Discussions, 2018, 211, 325-381.	1.6	7
52	Structure prediction of epitaxial inorganic interfaces by lattice and surface matching with OGRE. Journal of Chemical Physics, 2021, 155, 034111.	1.2	7
53	Electronic Structure of InAs and InSb Surfaces: Density Functional Theory and Angle-Resolved Photoemission Spectroscopy. Advanced Quantum Technologies, 2022, 5, .	1.8	6
54	Best practices for first-principles simulations of epitaxial inorganic interfaces. Journal of Physics Condensed Matter, 2022, 34, 233002.	0.7	6

#	ARTICLE	IF	CITATIONS
55	Performance of Dispersion-Inclusive Density Functional Theory Methods for Energetic Materials. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4456-4471.	2.3	6
56	Anomalous pressure dependence of the electronic properties of molecular crystals explained by changes in intermolecular electronic coupling. <i>Synthetic Metals</i> , 2019, 253, 9-19.	2.1	4
57	Finding predictive models for singlet fission by machine learning. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	4
58	Structure searching methods: general discussion. <i>Faraday Discussions</i> , 2018, 211, 133-180.	1.6	3
59	An energetics assessment of benzo[ <i>a</i> ]tetracene and benzo[ <i>a</i> ]pyrene as triplet-triplet annihilation emitters. <i>Molecular Systems Design and Engineering</i> , 2022, 7, 889-898.	1.7	2