Ismaila Dabo

List of Publications by Year
in descending order

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63 papers	20,374 citations	304743 22 h-index	114465 63 g-index
67 all docs	67 docs citations	67 times ranked	23363 citing authors

#	Article	IF	Citations
1	Surface reconstruction of oxidized platinum nanoparticles using classical molecular dynamics simulations. Computational Materials Science, 2022, 209, 111364.	3.0	2
2	Extensive Benchmarking of DFT+U Calculations for Predicting Band Gaps. Applied Sciences (Switzerland), 2021, 11, 2395.	2.5	75
3	Predicting the Pseudocapacitive Windows for MXene Electrodes with Voltage-Dependent Cluster Expansion Models. ACS Applied Energy Materials, 2021, 4, 3151-3159.	5.1	9
4	A promising Zn-Ti layered double hydroxide/Fe-bearing montmorillonite composite as an efficient photocatalyst for Cr(VI) reduction: Insight into the role of Fe impurity in montmorillonite. Applied Surface Science, 2021, 546, 148835.	6.1	30
5	Ferroelectricity in boron-substituted aluminum nitride thin films. Physical Review Materials, 2021, 5, .	2.4	53
6	Single-Step Direct Laser Writing of Multimetal Oxygen Evolution Catalysts from Liquid Precursors. ACS Nano, 2021, 15, 9796-9807.	14.6	11
7	Environmental impact of amino acids on the release of selenate immobilized in hydrotalcite: Integrated interpretation of experimental and density-functional theory study. Chemosphere, 2021, 274, 129927.	8.2	5
8	Quantifying multipoint ordering in alloys. Physical Review B, 2021, 104, .	3.2	2
9	Environmental impact of amino acids on selenate-bearing hydrocalumite: Experimental and DFT studies. Environmental Pollution, 2021, 288, 117687.	7.5	4
10	Optimizing accuracy and efficacy in data-driven materials discovery for the solar production of hydrogen. Energy and Environmental Science, 2021, 14, 2335-2348.	30.8	23
11	Data-driven analysis of the electronic-structure factors controlling the work functions of perovskite oxides. Physical Chemistry Chemical Physics, 2021, 23, 6880-6887.	2.8	7
12	Using C-DFT to develop an e-ReaxFF force field for acetophenone radical anion. Journal of Chemical Physics, 2021, 155, 214104.	3.0	1
13	Tuning Triplet-Pair Separation versus Relaxation Using a Diamond Anvil Cell. Cell Reports Physical Science, 2020, 1, 100005.	5.6	7
14	Spectroscopic and first-principles investigations of iodine species incorporation into ettringite: Implications for iodine migration in cement waste forms. Journal of Hazardous Materials, 2020, 389, 121880.	12.4	39
15	Colloidal Nanoparticles of a Metastable Copper Selenide Phase with Near-Infrared Plasmon Resonance. Chemistry of Materials, 2020, 32, 10227-10234.	6.7	19
16	Photophysics and Electronic Structure of Lateral Graphene/MoS₂ and Metal/MoS₂ Junctions. ACS Nano, 2020, 14, 16663-16671.	14.6	11
17	Phase-Selective Solution Synthesis of Perovskite-Related Cesium Cadmium Chloride Nanoparticles. Inorganic Chemistry, 2020, 59, 11688-11694.	4.0	30
18	First-principles study and experimental characterization of metal incorporation in germanium telluride. Journal of Applied Physics, 2020, 128, .	2.5	4

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19	Optimized utilization of COMB3 reactive potentials in LAMMPS. Journal of Chemical Physics, 2020, 152, 224702.	3.0	9
20	Achieving Minimal Heat Conductivity by Ballistic Confinement in Phononic Metalattices. ACS Nano, 2020, 14, 4235-4243.	14.6	14
21	Antisymmetry: Fundamentals and Applications. Annual Review of Materials Research, 2020, 50, 255-281.	9.3	9
22	Effects of surface charge and cluster size on the electrochemical dissolution of platinum nanoparticles using COMB3 and continuum electrolyte models. Journal of Chemical Physics, 2020, 152, 064102.	3.0	2
23	Electrochemical stability and light-harvesting ability of silicon photoelectrodes in aqueous environments. Journal of Chemical Physics, 2019, 151, 044109.	3.0	2
24	Understanding the influence of defects and surface chemistry on ferroelectric switching: a ReaxFF investigation of BaTiO₃. Physical Chemistry Chemical Physics, 2019, 21, 18240-18249.	2.8	45
25	MXene Electrode Materials for Electrochemical Energy Storage: First-Principles and Grand Canonical Monte Carlo Simulations. MRS Advances, 2019, 4, 1833-1841.	0.9	6
26	Vibrational probe of the origin of singlet exciton fission in TIPS-pentacene solutions. Journal of Chemical Physics, 2019, 151, 154701.	3.0	18
27	BaZrSe3: Ab initio study of anion substitution for bandgap tuning in a chalcogenide material. Journal of Applied Physics, 2019, 125, .	2.5	10
28	Topological Control of Water Reactivity on Glass Surfaces: Evidence of a Chemically Stable Intermediate Phase. Journal of Physical Chemistry Letters, 2019, 10, 3955-3960.	4.6	5
29	Implementation of distortion symmetry for the nudged elastic band method with DiSPy. Npj Computational Materials, 2019, 5, .	8.7	2
30	New frontiers for the materials genome initiative. Npj Computational Materials, 2019, 5, .	8.7	312
31	Conjugated Block Copolymers as Model Systems to Examine Mechanisms of Charge Generation in Donorâ€“Acceptor Materials. Advanced Functional Materials, 2019, 29, 1804858.	14.9	17
32	Voltage effects on the stability of Pd ensembles in Pdâ€“Au/Au(111) surface alloys. Journal of Chemical Physics, 2019, 150, 041715.	3.0	5
33	First-principles investigation of BiVO3 for thermochemical water splitting. International Journal of Hydrogen Energy, 2019, 44, 1425-1430.	7.1	6
34	Voltage-dependent reconstruction of layered <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Bi</mml:mi><mml:mn>2</mml:mn></mml:m and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Bi</mml:mi><mml:mn>2</mml:mn></mml:m photocatalysts and its influence on charge sepa. Physical Review Materials, 2019, 3, .	2.4	10
35	Influence of surface restructuring on the activity of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub><m photoelectrodes for photocatalytic hydrogen reduction. Physical Review Materials, 2019, 3, .	2.4	5
36	Probing the pseudocapacitance and energy-storage performance of RuO2 facets from first principles. Physical Review Materials, 2019, 3, .	2.4	6

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37	Discovering minimum energy pathways via distortion symmetry groups. Physical Review B, 2018, 98, .	3.2	14
38	Spatio-temporal symmetry â€“ crystallographic point groups with time translations and time inversion. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, 399-402.	0.1	6
39	Quantumâ€“continuum simulation of underpotential deposition at electrified metalâ€“solution interfaces. Npj Computational Materials, 2017, 3, .	8.7	88
40	A silicon microwire under a three-dimensional anisotropic tensile stress. Applied Physics Letters, 2017, 110, 091911.	3.3	0
41	Single-Crystal Silicon Optical Fiber by Direct Laser Crystallization. ACS Photonics, 2017, 4, 85-92.	6.6	43
42	Solution-Synthesized In4SnSe4 Semiconductor Microwires with a Direct Band Gap. Chemistry of Materials, 2017, 29, 1095-1098.	6.7	12
43	Triplet Transfer Mediates Triplet Pair Separation during Singlet Fission in 6,13â€Bis(triisopropylsilylethynyl)â€Pentacene. Advanced Functional Materials, 2017, 27, 1703929.	14.9	40
44	Quantum-continuum simulation of the electrochemical response of pseudocapacitor electrodes under realistic conditions. Physical Review B, 2017, 95, .	3.2	26
45	Quantum-continuum calculation of the surface states and electrical response of silicon in solution. Physical Review B, 2017, 95, .	3.2	16
46	Voltage-dependent cluster expansion for electrified solid-liquid interfaces: Application to the electrochemical deposition of transition metals. Physical Review B, 2017, 96, .	3.2	18
47	Removal mechanism of high concentration borate by co-precipitation with hydroxyapatite. Journal of Environmental Chemical Engineering, 2016, 4, 1092-1101.	6.7	16
48	Koopmans-Compliant Self-Interaction Corrections. Advances in Atomic, Molecular and Optical Physics, 2015, , 105-127.	2.3	5
49	First-Principles Photoemission Spectroscopy and Orbital Tomography in Molecules from Koopmans-Compliant Functionals. Physical Review Letters, 2015, 114, 166405.	7.8	38
50	Koopmans-compliant functionals and their performance against reference molecular data. Physical Review B, 2014, 90, .	3.2	81
51	Piecewise Linearity and Spectroscopic Properties from Koopmans-Compliant Functionals. Topics in Current Chemistry, 2014, 347, 193-233.	4.0	19
52	Bridging density-functional and many-body perturbation theory: Orbital-density dependence in electronic-structure functionals. Physical Review B, 2014, 89, .	3.2	32
53	Chemisorbed Molecules under Potential Bias: Detailed Insights from First-Principles Vibrational Spectroscopies. Electrochimica Acta, 2014, 121, 210-214.	5.2	22
54	Donor and acceptor levels of organic photovoltaic compounds from first principles. Physical Chemistry Chemical Physics, 2013, 15, 685-695.	2.8	36

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55	Resilience of gas-phase anharmonicity in the vibrational response of adsorbed carbon monoxide and breakdown under electrical conditions. Physical Review B, 2012, 86, .	3.2	6
56	Role of electronic localization in the phosphorescence of iridium sensitizing dyes. Journal of Chemical Physics, 2012, 137, 154309.	3.0	27
57	First-principles simulation of arsenate adsorption on the (1<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 677 Td (xmlns:mml surface of hematite. Geochimica Et Cosmochimica Acta, 2012, 86, 192-195.	3.9	40
58	Revised self-consistent continuum solvation in electronic-structure calculations. Journal of Chemical Physics, 2012, 136, 064102.	3.0	383
59	Electronic levels and electrical response of periodic molecular structures from plane-wave orbital-dependent calculations. Physical Review B, 2011, 84, .	3.2	19
60	Koopmansâ€™ condition for density-functional theory. Physical Review B, 2010, 82, .	3.2	206
61	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics Condensed Matter, 2009, 21, 395502.	1.8	18,183
62	Electrostatics in periodic boundary conditions and real-space corrections. Physical Review B, 2008, 77, .	3.2	116
63	Vibrational Recognition of Adsorption Sites for CO on Platinum and Platinumâ^'Ruthenium Surfaces. Journal of the American Chemical Society, 2007, 129, 11045-11052.	13.7	40