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	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
2	Revised self-consistent continuum solvation in electronic-structure calculations. Journal of Chemical Physics, 2012, 136, 064102.	3.0	383
3	New frontiers for the materials genome initiative. Npj Computational Materials, 2019, 5, .	8.7	312
4	Koopmansâ€™ condition for density-functional theory. Physical Review B, 2010, 82, .	3.2	206
5	Electrostatics in periodic boundary conditions and real-space corrections. Physical Review B, 2008, 77, .	3.2	116
6	Quantumâ€“continuum simulation of underpotential deposition at electrified metalâ€“solution interfaces. Npj Computational Materials, 2017, 3, .	8.7	88
7	Koopmans-compliant functionals and their performance against reference molecular data. Physical Review B, 2014, 90, .	3.2	81
8	Extensive Benchmarking of DFT+U Calculations for Predicting Band Gaps. Applied Sciences (Switzerland), 2021, 11, 2395.	2.5	75
9	Ferroelectricity in boron-substituted aluminum nitride thin films. Physical Review Materials, 2021, 5, .	2.4	53
10	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
11	Single-Crystal Silicon Optical Fiber by Direct Laser Crystallization. ACS Photonics, 2017, 4, 85-92.	6.6	43
12	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
13	First-principles simulation of arsenate adsorption on the (1<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 277 Td (xmlns:m surface of hematite. Geochimica Et Cosmochimica Acta, 2012, 86, 192-205.	3.9	40
14	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
15	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
16	First-Principles Photoemission Spectroscopy and Orbital Tomography in Molecules from Koopmans-Compliant Functionals. Physical Review Letters, 2015, 114, 166405.	7.8	38
17	Donor and acceptor levels of organic photovoltaic compounds from first principles. Physical Chemistry Chemical Physics, 2013, 15, 685-695.	2.8	36
18	Bridging density-functional and many-body perturbation theory: Orbital-density dependence in electronic-structure functionals. Physical Review B, 2014, 89, .	3.2	32

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19	Phase-Selective Solution Synthesis of Perovskite-Related Cesium Cadmium Chloride Nanoparticles. Inorganic Chemistry, 2020, 59, 11688-11694.	4.0	30
20	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
21	Role of electronic localization in the phosphorescence of iridium sensitizing dyes. Journal of Chemical Physics, 2012, 137, 154309.	3.0	27
22	Quantum-continuum simulation of the electrochemical response of pseudocapacitor electrodes under realistic conditions. Physical Review B, 2017, 95, .	3.2	26
23	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
24	Chemisorbed Molecules under Potential Bias: Detailed Insights from First-Principles Vibrational Spectroscopies. Electrochimica Acta, 2014, 121, 210-214.	5.2	22
25	Electronic levels and electrical response of periodic molecular structures from plane-wave orbital-dependent calculations. Physical Review B, 2011, 84, .	3.2	19
26	Piecewise Linearity and Spectroscopic Properties from Koopmans-Compliant Functionals. Topics in Current Chemistry, 2014, 347, 193-233.	4.0	19
27	Colloidal Nanoparticles of a Metastable Copper Selenide Phase with Near-Infrared Plasmon Resonance. Chemistry of Materials, 2020, 32, 10227-10234.	6.7	19
28	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
29	Vibrational probe of the origin of singlet exciton fission in TIPS-pentacene solutions. Journal of Chemical Physics, 2019, 151, 154701.	3.0	18
30	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
31	Removal mechanism of high concentration borate by co-precipitation with hydroxyapatite. Journal of Environmental Chemical Engineering, 2016, 4, 1092-1101.	6.7	16
32	Quantum-continuum calculation of the surface states and electrical response of silicon in solution. Physical Review B, 2017, 95, .	3.2	16
33	Discovering minimum energy pathways via distortion symmetry groups. Physical Review B, 2018, 98, .	3.2	14
34	Achieving Minimal Heat Conductivity by Ballistic Confinement in Phononic Metalattices. ACS Nano, 2020, 14, 4235-4243.	14.6	14
35	Solution-Synthesized In4SnSe4 Semiconductor Microwires with a Direct Band Gap. Chemistry of Materials, 2017, 29, 1095-1098.	6.7	12
36	Photophysics and Electronic Structure of Lateral Graphene/MoS₂ and Metal/MoS₂ Junctions. ACS Nano, 2020, 14, 16663-16671.	14.6	11

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37	Single-Step Direct Laser Writing of Multimetal Oxygen Evolution Catalysts from Liquid Precursors. ACS Nano, 2021, 15, 9796-9807.	14.6	11
38	BaZrSe3: Ab initio study of anion substitution for bandgap tuning in a chalcogenide material. Journal of Applied Physics, 2019, 125, .	2.5	10
39	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:msub></mml:mrow></mml:math> 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:msub></mml:mrow></mml:math> photocatalysts and its influence on charge sepa. Physical Review Materials, 2019, 3, .	2.4	10
40	Optimized utilization of COMB3 reactive potentials in LAMMPS. Journal of Chemical Physics, 2020, 152, 224702.	3.0	9
41	Antisymmetry: Fundamentals and Applications. Annual Review of Materials Research, 2020, 50, 255-281.	9.3	9
42	Predicting the Pseudocapacitive Windows for MXene Electrodes with Voltage-Dependent Cluster Expansion Models. ACS Applied Energy Materials, 2021, 4, 3151-3159.	5.1	9
43	Tuning Triplet-Pair Separation versus Relaxation Using a Diamond Anvil Cell. Cell Reports Physical Science, 2020, 1, 100005.	5.6	7
44	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
45	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
46	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
47	MXene Electrode Materials for Electrochemical Energy Storage: First-Principles and Grand Canonical Monte Carlo Simulations. MRS Advances, 2019, 4, 1833-1841.	0.9	6
48	First-principles investigation of BiVO3 for thermochemical water splitting. International Journal of Hydrogen Energy, 2019, 44, 1425-1430.	7.1	6
49	Probing the pseudocapacitance and energy-storage performance of RuO2 facets from first principles. Physical Review Materials, 2019, 3, .	2.4	6
50	Koopmans-Compliant Self-Interaction Corrections. Advances in Atomic, Molecular and Optical Physics, 2015, , 105-127.	2.3	5
51	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
52	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
53	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
54	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></mml:math> photoelectrodes for photocatalytic hydrogen reduction. Physical Review Materials, 2019, 3, .	2.4	5

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55	First-principles study and experimental characterization of metal incorporation in germanium telluride. Journal of Applied Physics, 2020, 128, .	2.5	4
56	Environmental impact of amino acids on selenate-bearing hydrocalumite: Experimental and DFT studies. Environmental Pollution, 2021, 288, 117687.	7.5	4
57	Electrochemical stability and light-harvesting ability of silicon photoelectrodes in aqueous environments. Journal of Chemical Physics, 2019, 151, 044109.	3.0	2
58	Implementation of distortion symmetry for the nudged elastic band method with DiSPy. Npj Computational Materials, 2019, 5, .	8.7	2
59	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
60	Quantifying multipoint ordering in alloys. Physical Review B, 2021, 104, .	3.2	2
61	Surface reconstruction of oxidized platinum nanoparticles using classical molecular dynamics simulations. Computational Materials Science, 2022, 209, 111364.	3.0	2
62	Using C-DFT to develop an e-ReaxFF force field for acetophenone radical anion. Journal of Chemical Physics, 2021, 155, 214104.	3.0	1
63	A silicon microwire under a three-dimensional anisotropic tensile stress. Applied Physics Letters, 2017, 110, 091911.	3.3	0