Mazharul M Islam

List of Publications by Year
in descending order

52	1,636	304701	302107
papers	citations	22 h-index	39 g-index

55	55	55	2377
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Theoretical Study of Li Migration in Lithiumâ€“Graphite Intercalation Compounds with Dispersion-Corrected DFT Methods. Journal of Physical Chemistry C, 2014, 118, 2273-2280.	3.1	141
2	Hydrogen Adsorption and Diffusion on the Anatase TiO₂(101) Surface: A First-Principles Investigation. Journal of Physical Chemistry C, 2011, 115, 6809-6814.	3.1	136
3	Electronic properties of oxygen-deficient and aluminum-doped rutile<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>from first principles. Physical Review B, 2007, 76, .	3.2	119
4	Characterization of Supported Vanadium Oxide Species on Silica: A Periodic DFT Investigation. Journal of Physical Chemistry C, 2009, 113, 10740-10746.	3.1	75
5	Bulk and surface properties of Cu2O: A first-principles investigation. Computational and Theoretical Chemistry, 2009, 903, 41-48.	1.5	67
6	Theoretical Analysis of Structural, Energetic, Electronic, and Defect Properties of Li2O. Journal of Physical Chemistry B, 2006, 110, 9413-9420.	2.6	66
7	Structural, Magnetic, Electronic, Defect, and Diffusion Properties of Cr₂O₃: A DFT+U Study. Journal of Physical Chemistry C, 2014, 118, 18133-18145.	3.1	66
8	Structural and Electronic Properties of Li2B4O7. Journal of Physical Chemistry B, 2005, 109, 13597-13604.	2.6	61
9	Ab initio study of the chemical states of water on Cr2O3(0001): From the isolated molecule to saturation coverage. Surface Science, 2009, 603, 2484-2493.	1.9	55
10	Density Functional Theory Study for the Stability and Ionic Conductivity of Li₂O Surfaces. Journal of Physical Chemistry C, 2009, 113, 672-676.	3.1	50
11	First principles investigation on the stabilization mechanisms of the polar copper terminated Cu2O(111) surface. Surface Science, 2009, 603, 2087-2095.	1.9	49
12	Unravelling Ultraslow Lithium-Ion Diffusion in Î³-LiAlO₂: Experiments with Tracers, Neutrons, and Charge Carriers. Chemistry of Materials, 2016, 28, 915-924.	6.7	49
13	Electronic properties of compounds of theLi2Oâ^'B2O3system. Physical Review B, 2005, 72, .	3.2	43
14	Dependence of pressure on elastic, electronic and optical properties of CeO2 and ThO2: A first principles study. Computational Materials Science, 2011, 50, 2280-2286.	3.0	36
15	Synergy between iono-covalent bonds and van der Waals interactions in SAMs formation: A first-principles study of adsorption of carboxylic acids on the Znâ€“ZnO(0001) surface. Catalysis Today, 2011, 177, 39-49.	4.4	34
16	Lithium Diffusion Pathways in Î²-Li₂TiO₃: A Theoretical Study. Journal of Physical Chemistry C, 2016, 120, 7061-7066.	3.1	34
17	Chlorine ion mobility in Cl-mayenite (Ca12Al14O32Cl2): An investigation combining high-temperature neutron powder diffraction, impedance spectroscopy and quantum-chemical calculations. Solid State Ionics, 2014, 254, 48-58.	2.7	33
18	Theoretical investigation of the nonlinear optical properties of substituted anilines and N,N-dimethylanilines. Computational and Theoretical Chemistry, 2011, 967, 165-170.	2.5	32

#	Article	IF	Citations
19	Interstitial Lithium Diffusion Pathways in Î³-LiAlO₂: A Computational Study. Journal of Physical Chemistry Letters, 2015, 6, 4622-4626.	4.6	29
20	Ionic Conductivity of Li2B4O7. Journal of Physical Chemistry B, 2006, 110, 17518-17523.	2.6	25
21	Comparison of trigonal B2O3 structures with high and low space-group symmetry. Chemical Physics Letters, 2006, 418, 565-568.	2.6	25
22	Electronic Properties of Vanadiumâ€Doped TiO₂. ChemPhysChem, 2011, 12, 3467-3473.	2.1	25
23	Electronic and optical properties of BAs under pressure. Physica B: Condensed Matter, 2011, 406, 4272-4277.	2.7	24
24	The ionic conductivity in lithium-boron oxide materials and its relation to structural, electronic and defect properties: insights from theory. Journal of Physics Condensed Matter, 2012, 24, 203201.	1.8	22
25	Enhanced Conductivity at the Interface of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Li</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mo>â^¶</mml:mo><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>Nanocomposites: At	7.8	20
26	Surface reconstruction modes of Cu2O(001) surface: A first principles study. Surface Science, 2010, 604, 1516-1523.	1.9	20
27	CN-mayenite Ca12Al14O32(CN)2: Replacing mobile oxygen ions by cyanide ions. Solid State Sciences, 2014, 38, 69-78.	3.2	20
28	Chromium sites in zeolite framework: Chromyl or chromium hydroxyl groups?. Microporous and Mesoporous Materials, 2012, 159, 66-73.	4.4	18
29	Atomistic Modeling of Voiding Mechanisms at Oxide/Alloy Interfaces. Journal of Physical Chemistry C, 2009, 113, 9978-9981.	3.1	17
30	Structural Analysis and Li Migration Pathways in Ramsdellite Li₂Ti₃O₇: A Theoretical Study. Journal of Physical Chemistry C, 2016, 120, 5-10.	3.1	17
31	The Effects of Oxidation States, Spin States and Solvents on Molecular Structure, Stability and Spectroscopic Properties of Fe-Catechol Complexes: A Theoretical Study. Advances in Chemical Engineering and Science, 2017, 07, 137-153.	0.5	17
32	Rutile Band-Gap States Induced by Doping with Manganese in Various Oxidation States. Journal of Physical Chemistry C, 2015, 119, 5534-5541.	3.1	16
33	Lithium Diffusion Pathways in 3R-Li_{<i>x</i>}TiS₂: A Combined Neutron Diffraction and Computational Study. Journal of Physical Chemistry C, 2015, 119, 11370-11381.	3.1	16
34	From Atoms to Cells: Multiscale Modeling of LiNi_{<i>x</i>}Mn_{<i>y</i>}Co_{<i>z</i>}O₂ Cathodes for Li-Ion Batteries. ACS Energy Letters, 2022, 7, 108-122.	17.4	16
35	Formation and Mobility of Li Point Defects in LiBO₂: A First-Principles Investigation. Journal of Physical Chemistry C, 2011, 115, 12343-12349.	3.1	15
36	Reconstruction of low-index graphite surfaces. Surface Science, 2016, 649, 60-65.	1.9	15

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37	The structure of reconstructed chalcopyrite surfaces. Surface Science, 2018, 669, 1-9.	1.9	15
38	Experimental and Theoretical Insights into Influence of Hydrogen and Nitrogen Plasma on the Water Splitting Performance of ALD Grown TiO₂ Thin Films. Journal of Physical Chemistry C, 2017, 121, 15538-15548.	3.1	13
39	Crystal Structure of 3Râ€LiTiS₂ and its Stability Compared to Other Polymorphs. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2013, 639, 2822-2825.	1.2	12
40	Pushing the boundaries of lithium battery research with atomistic modelling on different scales. Progress in Energy, 2022, 4, 012002.	10.9	12
41	Reconstruction of TiAl Intermetallic Surfaces: A Combined STM and DFT Study. Journal of Physical Chemistry C, 2011, 115, 3372-3377.	3.1	11
42	Theoretical study of low-index surfaces of trigonal B2O3. Surface Science, 2008, 602, 2217-2221.	1.9	10
43	Lithium Diffusion Mechanisms in Î²-LiMO₂ (M = Al, Ga): A Combined Experimental and Theoretical Study. Journal of Physical Chemistry C, 2017, 121, 27788-27796.	3.1	10
44	Insights into Li⁺ Migration Pathways in Î±-Li₃VF₆: A First-Principles Investigation. Journal of Physical Chemistry Letters, 2012, 3, 3120-3124.	4.6	9
45	Diffusion Pathways and Activation Energies in Crystalline Lithium-Ion Conductors. Zeitschrift Fur Physikalische Chemie, 2017, 231, 1279-1302.	2.8	9
46	Theoretical Investigation of Migration Pathways for Li Diffusion in h-LiTiS ₂ . Zeitschrift Fur Physikalische Chemie, 2012, 226, 449-459.	2.8	8
47	Zn effect on STM imaging of brass surfaces. Surface Science, 2016, 644, 148-152.	1.9	7
48	Stress Concentration in the Bulk Cr₂O₃: Effects of Temperature and Point Defects. Journal of Chemistry, 2017, 2017, 1-8.	1.9	6
49	Energy ordering of grain boundaries in Cr2O3: insights from theory. Journal of Physics Condensed Matter, 2013, 25, 485005.	1.8	5
50	Density Functional Theory Evaluated for Structural and Electronic Properties of 1T-Li_xTiS₂ and Lithium Ion Migration in 1T-Li_{0.94}TiS₂. Zeitschrift Fur Physikalische Chemie, 2017, 231, 1263-1278.	2.8	4
51	3D Li Diffusion in c-LixTiS2 (xâ€‰=â€‰0.69 and 0.75): A Theoretical Study. Zeitschrift Fur Physikalische Chemie, 2015, 229, 1265-1274.	2.8	2
52	Structural and Electronic Properties of Li2B4O7. ChemInform, 2005, 36, no.	0.0	0