Mohammad N Huda

List of Publications by Year
in descending order

107	3,419	159358 30	149479 56
papers	citations	h-index	g-index

108	108	108	4695
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Band Edge Electronic Structure of BiVO₄: Elucidating the Role of the Bi s and V d Orbitals. Chemistry of Materials, 2009, 21, 547-551.	3.2	624
2	Electrodeposited Aluminum-Doped Î±-Fe₂O₃ Photoelectrodes: Experiment and Theory. Chemistry of Materials, 2010, 22, 510-517.	3.2	240
3	Electronic structure, photovoltage, and photocatalytic hydrogen evolution with p-CuBi₂O₄ nanocrystals. Journal of Materials Chemistry A, 2016, 4, 2936-2942.	5.2	158
4	Electronic, structural, and magnetic effects of 3d transition metals in hematite. Journal of Applied Physics, 2010, 107, .	1.1	135
5	Electronic structure basis for enhanced overall water splitting photocatalysis with aluminum doped SrTiO₃ in natural sunlight. Energy and Environmental Science, 2019, 12, 1385-1395.	15.6	134
6	Band-Engineered Bismuth Titanate Pyrochlores for Visible Light Photocatalysis. Journal of Physical Chemistry C, 2010, 114, 10598-10605.	1.5	126
7	Tungsten-based oxide semiconductors for solar hydrogen generation. Catalysis Today, 2013, 199, 53-64.	2.2	123
8	Density-functional theory study of the effects of atomic impurity on the band edges of monoclinic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>WO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:ms Physical Review B, 2008, 77, .	1.1	93
9	Electronic structure of ZnO:GaN compounds: Asymmetric bandgap engineering. Physical Review B, 2008, 78, .	1.1	93
10	Effect of spin-orbit coupling on small platinum nanoclusters. Physical Review A, 2006, 73, .	1.0	83
11	Electronic structures and magic numbers of small silver clusters: A many-body perturbation-theoretic study. Physical Review A, 2003, 67, .	1.0	71
12	Group-IIIA versus IIIB delafossites: Electronic structure study. Physical Review B, 2009, 80, .	1.1	69
13	h-BNmonolayer adsorption on theNi(111)surface: A density functional study. Physical Review B, 2006, 74, .	1.1	61
14	Ternary cobalt spinel oxides for solar driven hydrogen production: Theory and experiment. Energy and Environmental Science, 2009, 2, 774.	15.6	60
15	Solution Combustion Synthesis, Characterization, and Photoelectrochemistry of CuNb₂O₆ and ZnNb₂O₆ Nanoparticles. Journal of Physical Chemistry C, 2016, 120, 16024-16034.	1.5	56
16	Evolution of SiC nanocluster from carbon fullerene: A density functional theoretic study. Chemical Physics Letters, 2008, 457, 124-129.	1.2	55
17	Enhancing the visible light absorbance of Bi2Ti2O7 through Fe-substitution and its effects on photocatalytic hydrogen evolution. Applied Catalysis B: Environmental, 2014, 144, 261-268.	10.8	53
18	Timeâ€•and Energyâ€Efficient Solution Combustion Synthesis of Binary Metal Tungstate Nanoparticles with Enhanced Photocatalytic Activity. ChemSusChem, 2015, 8, 1652-1663.	3.6	44

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19	Photoelectrochemical Properties and Behavior of Î±-SnWO₄ Photoanodes Synthesized by Hydrothermal Conversion of WO₃ Films. ACS Applied Materials & Interfaces, 2017, 9, 1459-1470.	4.0	42
20	A density functional study of atomic hydrogen adsorption on plutonium layers. Physica B: Condensed Matter, 2004, 352, 5-17.	1.3	39
21	On the existence of Siâ€“C double bonded graphene-like layers. Chemical Physics Letters, 2009, 479, 255-258.	1.2	39
22	Pinning of the Fermi Level in CuFeO₂ by Polaron Formation Limiting the Photovoltage for Photochemical Water Splitting. Advanced Functional Materials, 2020, 30, 1910432.	7.8	38
23	Mechanism Behind the Easy Exfoliation of Ga₂O₃ Ultraâ€Thin Film Along (100) Surface. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1800554.	1.2	36
24	Silicon-Carbide Nano-Clusters: A Pathway to Future Nano-Electronics. Journal of Computational and Theoretical Nanoscience, 2006, 3, 315-341.	0.4	36
25	Rapid One-Pot Synthesis and Photoelectrochemical Properties of Copper Vanadates. ACS Applied Energy Materials, 2019, 2, 2837-2847.	2.5	34
26	Density functional study of O2 adsorption on (100) surface of ?-uranium. International Journal of Quantum Chemistry, 2005, 102, 98-105.	1.0	33
27	Molecular hydrogen adsorption and dissociation on the plutonium (111) surface. Physical Review B, 2005, 72, .	1.1	32
28	A correlation study of small silver clusters. European Physical Journal D, 2003, 22, 217-227.	0.6	31
29	Electronic structures and bonding of oxygen on plutonium layers. European Physical Journal B, 2004, 40, 337-346.	0.6	31
30	Photocatalytic Generation of Syngas Using Combustionâ€Synthesized Silver Bismuth Tungstate. ChemPhysChem, 2012, 13, 2945-2955.	1.0	30
31	Morphology-dependent optical absorption and conduction properties of photoelectrochemical photocatalysts for H2 production: A case study. Journal of Applied Physics, 2010, 107, .	1.1	29
32	Carbon dimer in silicon cage: A class of highly stable silicon carbide clusters. Physical Review A, 2004, 69, .	1.0	28
33	Mott insulators: An early selection criterion for materials for photoelectrochemical H2 production. Journal of Renewable and Sustainable Energy, 2011, 3, .	0.8	27
34	Possible effects of oxygen in Te-rich Î£3 (112) grain boundaries in CdTe. Solid State Communications, 2012, 152, 1744-1747.	0.9	27
35	Phase-Pure Copper Vanadate (Î±-CuV₂O₆): Solution Combustion Synthesis and Characterization. Chemistry of Materials, 2020, 32, 6247-6255.	3.2	27
36	Hydrogen adsorption and dissociation on small platinum clusters: An electronic structure density functional study. Physical Review B, 2006, 74, .	1.1	26

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37	Predicting a new photocatalyst and its electronic properties by density functional theory. Journal of Applied Physics, 2013, 114, .	1.1	24
38	Theoretical limits on the stability of single-phase kesterite-Cu2ZnSnS4. Journal of Applied Physics, 2015, 117, .	1.1	22
39	Understanding the thermodynamic pathways of SnO-to-SnO x phase transition. Computational Materials Science, 2016, 111, 359-365.	1.4	22
40	The photon absorber and interconnecting layers in multijunction organic solar cell. Solar Energy, 2020, 201, 28-44.	2.9	22
41	Carbon Fibers Coated with Ternary Niâ€“Coâ€“Se Alloy Particles as a Low-Cost Counter Electrode for Flexible Dye Sensitized Solar Cells. ACS Applied Energy Materials, 2021, 4, 870-878.	2.5	22
42	A density functional study of molecular oxygen adsorption and reaction barrier on Pu (100) surface. European Physical Journal B, 2005, 43, 131-141.	0.6	21
43	An ab initio study of H2 interaction with the Pu (100) surface. Physica B: Condensed Matter, 2005, 366, 95-109.	1.3	20
44	Symmetry-breaking-induced enhancement of visible light absorption in delafossite alloys. Applied Physics Letters, 2009, 94, 251907.	1.5	20
45	Ab initio study of molecular oxygen adsorption on Pu (111) surface. International Journal of Quantum Chemistry, 2005, 105, 280-291.	1.0	19
46	The effects of Bi alloying in Cu delafossites: A density functional theory study. Journal of Applied Physics, 2011, 109, .	1.1	17
47	Free energy landscape approach to aid pure phase synthesis of transition metal (X=Cr, Mn and Fe) doped bismuth titanate (Bi2Ti2O7). Journal of Crystal Growth, 2016, 444, 46-54.	0.7	16
48	Electronic and optical properties of CoX2O4 (Xâ€‰=â€‰Al, Ga, In) alloys. Applied Physics Letters, 2012, 100, .	1.5	15
49	Exchange-induced negative-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>U</mml:mi></mml:math>charge order in N-doped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>WO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml: A spin-Peierls-like system. Physical Review B, 2009, 80, .	1.1	14
50	Atomic oxygen adsorption on 3.125 at.% Ga stabilized Î´-Pu (1 1 1) surface. Journal of Alloys and Compounds, 2015, 643, 253-262.	2.8	14
51	Niobium Doping in BiVO₄: Interplay Between Effective Mass, Stability, and Pressure. ChemPhysChem, 2019, 20, 773-784.	1.0	14
52	Silicon-Carbide Nanostructures to Nanotubes. Journal of Computational and Theoretical Nanoscience, 2007, 4, 739-744.	0.4	13
53	Band gap reduction of ZnO for photoelectrochemical splitting of water. Proceedings of SPIE, 2007, , .	0.8	12
54	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>DFT</mml:mtext><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math>s for the energy minimum among eight collinear and noncollinear magnetic structures of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>GdB</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:ms Physical Review B, 2008, 78, .	1.1	12

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55	Size effects on the electronic and magnetic properties of PuO 2 (111) surface. Journal of Nuclear Materials, 2016, 468, 37-45.	1.3	12
56	A new type of cuprous-cysteamine sensitizers: Synthesis, optical properties and potential applications. Materials Today Physics, 2021, 19, 100435.	2.9	12
57	Silicon-carbon fullerenelike nanostructures: Anab initiostudy on the stability ofSi60C2n(n=1, 2) clusters. Physical Review A, 2005, 72, .	1.0	11
58	Novel silicon-carbon fullerene-like cages. European Physical Journal D, 2004, 31, 63-68.	0.6	10
59	Stability enhancement of Cu₂S against Cu vacancy formation by Ag alloying. Journal of Physics Condensed Matter, 2018, 30, 165701.	0.7	10
60	Electrodeposition of Silver Vanadate Films: A Tale of Two Polymorphs. ChemPhysChem, 2019, 20, 2635-2646.	1.0	10
61	Mobility and clustering of barium ions and dications in high-pressure xenon gas. Physical Review A, 2018, 97, .	1.0	9
62	Prediction of a New Phase of CuxS near Stoichiometric Composition. International Journal of Photoenergy, 2015, 2015, 1-7.	1.4	8
63	Thermodynamic analysis of fuels in gas phase: ethanol, gasoline and ethanol â€" gasoline predicted by DFT method. Journal of Molecular Modeling, 2015, 21, 267.	0.8	8
64	Influence of Ga on H Reactivity with Ga-Stabilized Î´-Pu Alloys. Journal of Physical Chemistry C, 2017, 121, 19162-19172.	1.5	8
65	Synthesis and optoelectronic properties of a promising quaternary metal oxide light absorber CuBiW₂O₈. Journal of Materials Chemistry A, 2021, 9, 1643-1654.	5.2	8
66	A density functional theoretic study of novel silicon-carbon fullerene-like nanostructures: Si40C20, Si60C20, Si36C24, and Si60C24. European Physical Journal D, 2006, 39, 227-236.	0.6	7
67	Understanding oxygen adsorption on 9.375 at. % Ga-stabilized Î´-Pu (111) surface: A DFT study. Journal of Alloys and Compounds, 2015, 653, 411-421.	2.8	7
68	Theoretical studies on the energy structures and optical properties of copper cysteamine â€“ a novel sensitizer. Physical Chemistry Chemical Physics, 2019, 21, 21084-21093.	1.3	7
69	First-principles study on the effect of Sn doping in Cu2Sâ€"Acanthite phase as a substitute to low chalcocite for modeling complex doping. Journal of Applied Physics, 2020, 128, .	1.1	7
70	Strong asymmetrical doping properties of spinel CoAl2O4. Journal of Applied Physics, 2012, 111, 093723.	1.1	6
71	Electronic Properties of SbTa₁₋_xNb_xO₄: Phase-Related Distortions. Journal of the Electrochemical Society, 2019, 166, H3195-H3201.	1.3	6
72	Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations. Heliyon, 2019, 5, e02908.	1.4	6

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73	Application of attractive potential by DFT+U to predict the electronic properties of materials without highly localized bands. Computational Materials Science, 2014, 81, 290-295.	1.4	5
74	The effect of noble metals in Si nanocrystals. Chemical Physics Letters, 2014, 605-606, 38-43.	1.2	5
75	Free energy dependence of pure phase iron doped bismuth titanate from first principles calculations. Journal of Physics Condensed Matter, 2015, 27, 315502.	0.7	5
76	One-step hydrogen extraction and storage in plasma generated palladium nanoparticles. Journal of Nanoparticle Research, 2018, 20, 1.	0.8	5
77	SiC Nanostructures from a Theoretical Perspective. Reviews in Nanoscience and Nanotechnology, 2014, 3, 88-106.	0.4	5
78	Delafossite-alloy photoelectrodes for PEC hydrogen production: a density functional theory study. Proceedings of SPIE, 2010, , .	0.8	4
79	Theoretical Study of SiC Nanostructures: Current Status and a New Theoretical Approach. Journal of Computational and Theoretical Nanoscience, 2012, 9, 1881-1905.	0.4	4
80	The delocalized nature of holes in (Ga, N) cluster-doped ZnO. Journal of Physics Condensed Matter, 2012, 24, 415503.	0.7	4
81	The effect of hydrogen passivation on Si nanocrystals: Surface and spin states. Computational and Theoretical Chemistry, 2013, 1019, 125-131.	1.1	4
82	Electronic structure study of N, O related defects in GaP for photoelectrochemical applications. Journal of Materials Chemistry A, 2013, 1, 8425.	5.2	4
83	Thermodynamic DFT analysis of natural gas. Journal of Molecular Modeling, 2017, 23, 224.	0.8	4
84	Editorial: Carbon- and Inorganic-Based Nanostructures for Energy Applications. Frontiers in Materials, 2020, 7, .	1.2	4
85	BiSbWO6: Properties of a mixed 5s/6s lone-pair-electron system. Chemical Physics, 2021, 544, 111117.	0.9	4
86	Optical, Electrochemical, and Photoelectrochemical Behavior of Copper Pyrovanadate: A Unified Theoretical and Experimental Study. Journal of Physical Chemistry C, 2021, 125, 19609-19620.	1.5	4
87	Surface and Optoelectronic Properties of Ultrathin Trigonal Selenium: A Density Functional Theory Study with van der Waals Correction. Langmuir, 2022, 38, 8485-8494.	1.6	4
88	Nanobiology Think Tank: Computational and Theoretical Nanoscience is Taking off at the National Cancer Institute. Journal of Computational and Theoretical Nanoscience, 2006, 3, 599-602.	0.4	3
89	Predicting a quaternary tungsten oxide for sustainable photovoltaic application by density functional theory. Applied Physics Letters, 2015, 107, 233902.	1.5	2
90	Molecular Dynamics of H₂ Storage in Carbon Nanotubes Under External Electric Field Effects: A Sensor Proposal. Journal of Nanoscience and Nanotechnology, 2017, 17, 4858-4863.	0.9	2

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91	Role of f Electrons in the Optical and Photoelectrochemical Behavior of Ca(La_{1â€“x}Ce_x)₂S₄ (0 â‰¤ x â‰¤ 1). Inorganic Chemistry, 2019, 58, 4553-4560.	1.9	2
92	Photovoltaic Materials Design by Computational Studies: Metal Sulfides. , 2020, , 123-138.		2
93	Perspectiveâ€”Multinary Oxide Semiconductors for Solar Fuels Generation: Closing the Performance Gap between Theory and Practice. ECS Journal of Solid State Science and Technology, 2022, 11, 053001.	0.9	2
94	Anomalous Dependence of Band Gaps of Binary Nanotubes on Diameters. Journal of Computational and Theoretical Nanoscience, 2011, 8, 1502-1508.	0.4	1
95	Development of metal tungstate alloys for photoelectrochemical water splitting. Proceedings of SPIE, 2013, , .	0.8	1
96	Weakening of Si Si bonding in exohydrogenated Si60 nanoclusters. Chemical Physics Letters, 2017, 684, 60-66.	1.2	1
97	Low-Index Stoichiometric Surfaces of CuBiW2O8. Surface Science, 2021, 705, 121762.	0.8	1
98	Role of f-electrons in determining insulator to metal phase transitions of Ca(La1â^'xCex)2S4 (0â€‰â‰€â€‰xâ€‰â‰€â€‰1) solid solution: A DFTâ€‰+â€‰U study. Journal of Applied Physics, 2021, 130, 145102.	1.1	1
99	Determination of thermodynamic growth conditions for a high-efficiency Cu <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e1705" altimg="si10.svg"><mml:msub><mml:mrow		