Mohammad N Huda

List of Publications by Year in Descending Order

98 papers	2,828 citations	27 h-index	51 g-index
108 ext. papers	3,131 ext. citations	4.4 avg, IF	5.27 L-index

#	Paper	IF	Citations
98	Determination of thermodynamic growth conditions for a high-efficiency Cu2ZnSn(S1−xSe. *Computational Materials Science*, **2022**, 208, 111313	3.2	1
97	Role of f-electrons in determining insulator to metal phase transitions of Ca(La1−xCex)2S4 (0 ≤ x ≤ 1) solid solution: A DFT + U study. *Journal of Applied Physics*, **2021**, 130, 145102	2.5	0
96	BiSbWO6: Properties of a mixed 5s/6s lone-pair-electron system. *Chemical Physics*, **2021**, 544, 111117	2.3	0
95	Low-Index Stoichiometric Surfaces of CuBiW2O8. *Surface Science*, **2021**, 705, 121762	1.8	0
94	Synthesis and optoelectronic properties of a promising quaternary metal oxide light absorber CuBiW2O8. *Journal of Materials Chemistry A*, **2021**, 9, 1643-1654	13	2
93	Carbon Fibers Coated with Ternary NiCoSe Alloy Particles as a Low-Cost Counter Electrode for Flexible Dye Sensitized Solar Cells. *ACS Applied Energy Materials*, **2021**, 4, 870-878	6.1	7
92	A new type of cuprous-cysteamine sensitizers: Synthesis, optical properties and potential applications. *Materials Today Physics*, **2021**, 19, 100435	8	7
91	Optical, Electrochemical, and Photoelectrochemical Behavior of Copper Pyrovanadate: A Unified Theoretical and Experimental Study. *Journal of Physical Chemistry C*, **2021**, 125, 19609-19620	3.8	2
90	The photon absorber and interconnecting layers in multijunction organic solar cell. *Solar Energy*, **2020**, 201, 28-44	6.8	13
89	Phase-Pure Copper Vanadate (CuV2O6): Solution Combustion Synthesis and Characterization. *Chemistry of Materials*, **2020**, 32, 6247-6255	9.6	15
88	Pinning of the Fermi Level in CuFeO2 by Polaron Formation Limiting the Photovoltage for Photochemical Water Splitting. *Advanced Functional Materials*, **2020**, 30, 1910432	15.6	23
87	BiSbWO6: Band Energies Tuning of a Mixed Sb(5s)/Bi(6s) Lone-Pair-Electrons System. *ECS Meeting Abstracts*, **2020**, MA2020-02, 3837-3837	0	
86	Photovoltaic Materials Design by Computational Studies: Metal Sulfides **2020**, 123-138		2
85	First-principles study on the effect of Sn doping in Cu2SnS3 canthite phase as a substitute to low chalcocite for modeling complex doping. *Journal of Applied Physics*, **2020**, 128, 015703	2.5	5
84	Theoretical studies on the energy structures and optical properties of copper cysteamine - a novel sensitizer. *Physical Chemistry Chemical Physics*, **2019**, 21, 21084-21093	3.6	4
83	Rapid One-Pot Synthesis and Photoelectrochemical Properties of Copper Vanadates. *ACS Applied Energy Materials*, **2019**, 2, 2837-2847	6.1	22
82	Role of f Electrons in the Optical and Photoelectrochemical Behavior of Ca(LaCe)S (0 ≤ x ≤ 1). *Inorganic Chemistry*, **2019**, 58, 4553-4560	5.1	2

81	Electronic Properties of SbTa1-xNbxO4: Phase-Related Distortions. *Journal of the Electrochemical Society*, **2019**, 166, H3195-H3201	3.9	2
80	Electronic structure basis for enhanced overall water splitting photocatalysis with aluminum doped SrTiO3 in natural sunlight. *Energy and Environmental Science*, **2019**, 12, 1385-1395	35.4	73
79	Electrodeposition of Silver Vanadate Films: A Tale of Two Polymorphs. *ChemPhysChem*, **2019**, 20, 2635-2646	3.2	6
78	Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations. *Heliyon*, **2019**, 5, e02908	3.6	4
77	Mechanism Behind the Easy Exfoliation of Ga2O3 Ultra-Thin Film Along (100) Surface. *Physica Status Solidi - Rapid Research Letters*, **2019**, 13, 1800554	2.5	25
76	Niobium Doping in BiVO : Interplay Between Effective Mass, Stability, and Pressure. *ChemPhysChem* , **2019**, 20, 773-784	3.2	7
75	Stability enhancement of CuS against Cu vacancy formation by Ag alloying. *Journal of Physics Condensed Matter*, **2018**, 30, 165701	1.8	7
74	One-step hydrogen extraction and storage in plasma generated palladium nanoparticles. *Journal of Nanoparticle Research*, **2018**, 20, 1	2.3	3
73	Mobility and clustering of barium ions and dications in high-pressure xenon gas. *Physical Review A*, **2018**, 97,	2.6	6
72	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	1.3	2
71	Photoelectrochemical Properties and Behavior of □SnWO Photoanodes Synthesized by Hydrothermal Conversion of WO Films. *ACS Applied Materials & Interfaces*, **2017**, 9, 1459-1470	9.5	36
70	Influence of Ga on H Reactivity with Ga-Stabilized □Pu Alloys. *Journal of Physical Chemistry C*, **2017**, 121, 19162-19172	3.8	5
69	Thermodynamic DFT analysis of natural gas. *Journal of Molecular Modeling*, **2017**, 23, 224	2	4
68	Weakening of Si Si bonding in exohydrogenated Si60 nanoclusters. *Chemical Physics Letters*, **2017**, 684, 60-66	2.5	0
67	Solution Combustion Synthesis, Characterization, and Photoelectrochemistry of CuNb2O6 and ZnNb2O6 Nanoparticles. *Journal of Physical Chemistry C*, **2016**, 120, 16024-16034	3.8	45
66	Electronic structure, photovoltage, and photocatalytic hydrogen evolution with p-CuBi2O4 nanocrystals. *Journal of Materials Chemistry A*, **2016**, 4, 2936-2942	13	122
65	Understanding the thermodynamic pathways of SnO-to-SnO x phase transition. *Computational Materials Science*, **2016**, 111, 359-365	3.2	19
64	Size effects on the electronic and magnetic properties of PuO 2 (111) surface. *Journal of Nuclear Materials*, **2016**, 468, 37-45	3.3	8

63	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	1.6	14
62	Atomic oxygen adsorption on 3.125 at.% Ga stabilized δ-Pu (1 1 1) surface. *Journal of Alloys and Compounds*, **2015**, 643, 253-262	5.7	11
61	Free energy dependence of pure phase iron doped bismuth titanate from first principles calculations. *Journal of Physics Condensed Matter*, **2015**, 27, 315502	1.8	4
60	Thermodynamic analysis of fuels in gas phase: ethanol, gasoline and ethanol - gasoline predicted by DFT method. *Journal of Molecular Modeling*, **2015**, 21, 267	2	6
59	Understanding oxygen adsorption on 9.375 at. % Ga-stabilized δ-Pu (111) surface: A DFT study. *Journal of Alloys and Compounds*, **2015**, 653, 411-421	5.7	5
58	Predicting a quaternary tungsten oxide for sustainable photovoltaic application by density functional theory. *Applied Physics Letters*, **2015**, 107, 233902	3.4	1
57	Time- and energy-efficient solution combustion synthesis of binary metal tungstate nanoparticles with enhanced photocatalytic activity. *ChemSusChem*, **2015**, 8, 1652-63	8.3	38
56	Prediction of a New Phase of CuxS near Stoichiometric Composition. *International Journal of Photoenergy*, **2015**, 2015, 1-7	2.1	8
55	Theoretical limits on the stability of single-phase kesterite-Cu2ZnSnS4. *Journal of Applied Physics*, **2015**, 117, 035702	2.5	20
54	The effect of noble metals in Si nanocrystals. *Chemical Physics Letters*, **2014**, 605-606, 38-43	2.5	4
53	The possibility of optical excitations at the smallest gap of Cu-delafossite nanocrystals. *Journal Physics D: Applied Physics*, **2014**, 47, 405301	3	
52	Theoretical Modeling of Oxide-Photocatalysts for PEC Water Splitting. *Nanostructure Science and Technology*, **2014**, 113-134	0.9	
51	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	21.8	46
50	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	3.2	5
49	SiC Nanostructures from a Theoretical Perspective. *Reviews in Nanoscience and Nanotechnology*, **2014**, 3, 88-106		4
48	The effect of hydrogen passivation on Si nanocrystals: Surface and spin states. *Computational and Theoretical Chemistry*, **2013**, 1019, 125-131	2	3
47	Predicting a new photocatalyst and its electronic properties by density functional theory. *Journal of Applied Physics*, **2013**, 114, 133508	2.5	20
46	Electronic structure study of N, O related defects in GaP for photoelectrochemical applications. *Journal of Materials Chemistry A*, **2013**, 1, 8425	13	4

45	Tungsten-based oxide semiconductors for solar hydrogen generation. *Catalysis Today*, **2013**, 199, 53-64	5.3	109
44	Development of metal tungstate alloys for photoelectrochemical water splitting **2013**,		1
43	Theoretical Study of SiC Nanostructures: Current Status and a New Theoretical Approach. *Journal of Computational and Theoretical Nanoscience*, **2012**, 9, 1881-1905	0.3	2
42	Electronic and optical properties of CoX2O4 (X = Al, Ga, In) alloys. *Applied Physics Letters*, **2012**, 100, 023901	3.4	14
41	Possible effects of oxygen in Te-rich Σ3 (112) grain boundaries in CdTe. *Solid State Communications*, **2012**, 152, 1744-1747	1.6	25
40	Strong asymmetrical doping properties of spinel CoAl2O4. *Journal of Applied Physics*, **2012**, 111, 093723	2.5	3
39	The delocalized nature of holes in (Ga, N) cluster-doped ZnO. *Journal of Physics Condensed Matter*, **2012**, 24, 415503	1.8	4
38	Photocatalytic generation of syngas using combustion-synthesized silver bismuth tungstate. *ChemPhysChem*, **2012**, 13, 2945-55	3.2	27
37	The effects of Bi alloying in Cu delafossites: A density functional theory study. *Journal of Applied Physics*, **2011**, 109, 113710	2.5	15
36	Mott insulators: An early selection criterion for materials for photoelectrochemical H2 production. *Journal of Renewable and Sustainable Energy*, **2011**, 3, 053101	2.5	22
35	Electronic, structural, and magnetic effects of 3d transition metals in hematite. *Journal of Applied Physics*, **2010**, 107, 123712	2.5	111
34	Morphology-dependent optical absorption and conduction properties of photoelectrochemical photocatalysts for H2 production: A case study. *Journal of Applied Physics*, **2010**, 107, 123703	2.5	27
33	Band-Engineered Bismuth Titanate Pyrochlores for Visible Light Photocatalysis. *Journal of Physical Chemistry C*, **2010**, 114, 10598-10605	3.8	100
32	Electrodeposited Aluminum-Doped α-Fe2O3 Photoelectrodes: Experiment and Theory. *Chemistry of Materials*, **2010**, 22, 510-517	9.6	207
31	Delafossite-alloy photoelectrodes for PEC hydrogen production: a density functional theory study **2010**,		3
30	Exchange-induced negative-U charge order in N-doped WO3: A spin-Peierls-like system. *Physical Review B*, **2009**, 80,	3.3	14
29	Group-IIIA versus IIIB delafossites: Electronic structure study. *Physical Review B*, **2009**, 80,	3.3	60
28	Symmetry-breaking-induced enhancement of visible light absorption in delafossite alloys. *Applied Physics Letters*, **2009**, 94, 251907	3.4	19

27	On the existence of SiC double bonded graphene-like layers. *Chemical Physics Letters*, **2009**, 479, 255-258	2.5	36
26	Band Edge Electronic Structure of BiVO4: Elucidating the Role of the Bi s and V d Orbitals. *Chemistry of Materials*, **2009**, 21, 547-551	9.6	542
25	Ternary cobalt spinel oxides for solar driven hydrogen production: Theory and experiment. *Energy and Environmental Science*, **2009**, 2, 774	35.4	55
24	Density-functional theory study of the effects of atomic impurity on the band edges of monoclinic WO3. *Physical Review B*, **2008**, 77,	3.3	80
23	Electronic structure of ZnO:GaN compounds: Asymmetric bandgap engineering. *Physical Review B*, **2008**, 78,	3.3	85
22	DFT+U search for the energy minimum among eight collinear and noncollinear magnetic structures of GdB4. *Physical Review B*, **2008**, 78,	3.3	12
21	Evolution of SiC nanocluster from carbon fullerene: A density functional theoretic study. *Chemical Physics Letters*, **2008**, 457, 124-129	2.5	48
20	Band gap reduction of ZnO for photoelectrochemical splitting of water **2007**,		11
19	Silicon-Carbide Nanostructures to Nanotubes. *Journal of Computational and Theoretical Nanoscience*, **2007**, 4, 739-744	0.3	13
18	h-BN monolayer adsorption on the Ni(111) surface: A density functional study. *Physical Review B*, **2006**, 74,	3.3	56
17	Hydrogen adsorption and dissociation on small platinum clusters: An electronic structure density functional study. *Physical Review B*, **2006**, 74,	3.3	22
16	Effect of spin-orbit coupling on small platinum nanoclusters. *Physical Review A*, **2006**, 73,	2.6	72
15	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	0.3	3
14	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	1.3	6
13	Silicon-Carbide Nano-Clusters: A Pathway to Future Nano-Electronics. *Journal of Computational and Theoretical Nanoscience*, **2006**, 3, 315-341	0.3	28
12	An ab initio study of H2 interaction with the Pu (1 0 0) surface. *Physica B: Condensed Matter*, **2005**, 366, 95-109	2.8	18
11	A density functional study of molecular oxygen adsorption and reaction barrier on Pu (100) surface. *European Physical Journal B*, **2005**, 43, 131-141	1.2	20
10	Density functional study of O2 adsorption on (100) surface of uranium. *International Journal of Quantum Chemistry*, **2005**, 102, 98-105	2.1	27

9	Ab initio study of molecular oxygen adsorption on Pu (111) surface. *International Journal of Quantum Chemistry*, **2005**, 105, 280-291	2.1	16
8	Silicon-carbon fullerenelike nanostructures: An ab initio study on the stability of Si60C2n (n=1, 2) clusters. *Physical Review A*, **2005**, 72,	2.6	10
7	Molecular hydrogen adsorption and dissociation on the plutonium (111) surface. *Physical Review B*, **2005**, 72,	3.3	31
6	Carbon dimer in silicon cage: A class of highly stable silicon carbide clusters. *Physical Review A*, **2004** , 69,	2.6	27
5	Electronic structures and bonding of oxygen on plutonium layers. *European Physical Journal B*, **2004** , 40, 337-346	1.2	28
4	Novel silicon-carbon fullerene-like cages. *European Physical Journal D*, **2004**, 31, 63-68	1.3	9
3	A density functional study of atomic hydrogen adsorption on plutonium layers. *Physica B: Condensed Matter*, **2004**, 352, 5-17	2.8	35
2	A correlation study of small silver clusters. *European Physical Journal D*, **2003**, 22, 217-227	1.3	29
1	Electronic structures and magic numbers of small silver clusters: A many-body perturbation-theoretic study. *Physical Review A*, **2003**, 67,	2.6	68