

Rashid Ahmad

List of Publications by Year in descending order

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78
papers

1,946
citations

257450

24
h-index

276875

41
g-index

79
all docs

79
docs citations

79
times ranked

2261
citing authors

#	ARTICLE	IF	CITATIONS
1	Structural, electronic and optical properties of CsPbX ₃ (X=Cl, Br, I) for energy storage and hybrid solar cell applications. <i>Journal of Alloys and Compounds</i> , 2017, 705, 828-839.	5.5	203
2	Microporous Coordination Polymers As Selective Sorbents for Liquid Chromatography. <i>Langmuir</i> , 2009, 25, 11977-11979.	3.5	170
3	<i>Ab initio</i> study of the bandgap engineering of Al _{1-x} Ga _x N for optoelectronic applications. <i>Journal of Applied Physics</i> , 2011, 109, .	2.5	167
4	Liquid phase separations by crystalline microporous coordination polymers. <i>Chemical Science</i> , 2010, 1, 293.	7.4	161
5	Adsorptive removal of Cd ²⁺ from aqueous solutions by a highly stable covalent triazine-based framework. <i>New Journal of Chemistry</i> , 2018, 42, 10234-10242.	2.8	66
6	Electronic Band Structures of the Highly Desirable III-V Semiconductors: TB-mBJ DFT Studies. <i>Journal of Electronic Materials</i> , 2016, 45, 3314-3323.	2.2	54
7	The potential of cost-effective coconut husk for the removal of toxic metal ions for environmental protection. <i>Journal of Environmental Management</i> , 2006, 81, 286-295.	7.8	52
8	A comparative study of the removal of Cr(VI) from synthetic solution using natural biosorbents. <i>New Journal of Chemistry</i> , 2017, 41, 10799-10807.	2.8	47
9	Cr-Doped III-V Nitrides: Potential Candidates for Spintronics. <i>Journal of Electronic Materials</i> , 2011, 40, 1428-1436.	2.2	43
10	The use of functionalized aerogels as a low level chromium scavenger. <i>Microporous and Mesoporous Materials</i> , 2015, 203, 8-16.	4.4	43
11	Antiperovskite compounds SbNSr ₃ and BiNSr ₃ : Potential candidates for thermoelectric renewable energy generators. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2015, 379, 206-210.	2.1	40
12	Sawdust: Cost Effective Scavenger for the Removal of Chromium(III) Ions from Aqueous Solutions. <i>Water, Air, and Soil Pollution</i> , 2005, 163, 169-183.	2.4	36
13	Orientationally engineered 2D/3D perovskite for high efficiency solar cells. <i>Sustainable Energy and Fuels</i> , 2020, 4, 324-330.	4.9	35
14	Silica-based nanomaterials as designer adsorbents to mitigate emerging organic contaminants from water matrices. <i>Journal of Water Process Engineering</i> , 2020, 38, 101675.	5.6	33
15	Electronic Properties of Antiperovskite Materials from State-of-the-Art Density Functional Theory. <i>Journal of Chemistry</i> , 2015, 2015, 1-11.	1.9	32
16	Structural, microwave permittivity, and complex impedance studies of cation (Cr, Bi, Al, In) substituted SrNi-X hexagonal nano-sized ferrites. <i>Ceramics International</i> , 2020, 46, 1907-1915.	4.8	32
17	Removal of azo dye from aqueous solution by a low-cost activated carbon prepared from coal: adsorption kinetics, isotherms study, and DFT simulation. <i>Environmental Science and Pollution Research</i> , 2021, 28, 10234-10247.	5.3	30
18	Silicon carbide and III-Nitrides nanosheets: Promising anodes for Mg-ion batteries. <i>Materials Chemistry and Physics</i> , 2021, 257, 123785.	4.0	29

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19	Influence of electric field on CO ₂ removal by P-doped C ₆₀ -fullerene: A DFT study. <i>Chemical Physics Letters</i> , 2020, 742, 137155.	2.6	28
20	Investigation of half metallicity in Fe doped CdSe and Co doped CdSe materials. <i>Current Applied Physics</i> , 2012, 12, 184-187.	2.4	27
21	Modification of sludge-based biochar using air roasting-oxidation and its performance in adsorption of uranium(VI) from aqueous solutions. <i>Journal of Colloid and Interface Science</i> , 2022, 614, 547-555.	9.4	26
22	Effect of polyfunctional monomers on properties of radiation crosslinked EPDM/waste tire dust blend. <i>Radiation Physics and Chemistry</i> , 2012, 81, 421-425.	2.8	25
23	Density functional theory study of emerging pollutants removal from water by covalent triazine based framework. <i>Journal of Molecular Liquids</i> , 2020, 309, 113008.	4.9	25
24	Influence of Cr and Zn substitution on structural, magnetic and dielectric properties of Sr _{2-x} Zn _x Ni ₂ Fe _{28-y} Cr _y O ₄₆ X-type hexagonal ferrite. <i>Solid State Sciences</i> , 2020, 100, 106090.	3.2	24
25	Nano-porous C ₄ N as a toxic pesticide's scavenger: A quantum chemical approach. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 111, 108078.	2.4	24
26	A Bifunctional and Free-Standing Organic Composite Film with High Flexibility and Good Tensile Strength for Tribological and Electrochemical Applications. <i>Advanced Materials Technologies</i> , 2019, 4, 1900617.	5.8	21
27	Investigation of sorption of Hg(II) ions onto coconut husk from aqueous solution using radiotracer technique. <i>Radiochimica Acta</i> , 2003, 91, 533-538.	1.2	20
28	Influence of sepiolite and electron beam irradiation on the structural and physicochemical properties of polyethylene/starch nanocomposites. <i>Polymer Composites</i> , 2013, 34, 408-416.	4.6	20
29	Thermoelectric properties of metallic antiperovskites AXD ₃ (A=Ge, Sn, Pb, Al, Zn, Ga; X=N, C; D=Ca, Fe). <i>Tj ETQq1 1,0,784314,rgBT /Ove</i>	2.2	19
30	Temperature effected sorption of europium(III) onto 1-(2-pyridylazo)-2-naphthol impregnated polyurethane foam. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2005, 267, 147-153.	1.5	18
31	Tunable relativistic quasiparticle electronic and excitonic behavior of the FAPb(I _{1-x} Br _x) ₃ alloy. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 11943-11955.	2.8	18
32	Selective adsorption of CO ₂ from gas mixture by P-decorated C ₂₄ N ₂₄ fullerene assisted by an electric field: A DFT approach. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 103, 107806.	2.4	18
33	Structural features and dielectric behavior of Al substituted Cu _{0.7} Ni _{0.3} Fe ₂ O ₄ ferrites. <i>Materials Chemistry and Physics</i> , 2021, 273, 125028.	4.0	17
34	Pollution Problem in River Kabul: Accumulation Estimates of Heavy Metals in Native Fish Species. <i>BioMed Research International</i> , 2015, 2015, 1-7.	1.9	16
35	DFT studies of thermoelectric properties of Au intermetallics at 300 K. <i>Journal of Rare Earths</i> , 2018, 36, 197-202.	4.8	16
36	Penta graphene: a superior anode material for Mg-ion batteries with high specific theoretical capacity. <i>Ionics</i> , 2021, 27, 4819-4828.	2.4	15

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37	Adsorption modeling and thermodynamic characteristics of uranium(VI) ions onto 1-(2-pyridylazo)-2-naphthol (PAN) supported polyurethane foam. <i>Radiochimica Acta</i> , 2005, 93, 333-339.	1.2	14
38	Novel nitrogen-doped KFeS ₂ /C composites for the efficient removal of Cr(VI). <i>Environmental Science: Nano</i> , 2021, 8, 1057-1066.	4.3	14
39	Prevalence, molecular diagnosis and treatment of <i>Mycoplasma conjunctivae</i> isolated from infectious keratoconjunctivitis affected Lohi sheep maintained at Livestock Experiment Station, Bahadurnagar, Okara, Pakistan. <i>Tropical Animal Health and Production</i> , 2013, 45, 737-742.	1.4	13
40	First principle studies of electronic and magnetic properties of Lanthanide-Gold (RAu) binary intermetallics. <i>Journal of Magnetism and Magnetic Materials</i> , 2017, 422, 458-463.	2.3	13
41	Desulfurization of Lakhra coal by combined leaching and catalytic oxidation techniques. <i>International Journal of Coal Preparation and Utilization</i> , 2022, 42, 124-140.	2.1	13
42	Study on influence of catalysts on product distribution during liquefaction of Pakistani coal. <i>Energy Conversion and Management</i> , 2007, 48, 2502-2507.	9.2	12
43	Removal of Traces of Silver Ions from Aqueous Solutions Using Coconut Husk as a Sorbent. <i>Separation Science and Technology</i> , 2005, 39, 3509-3525.	2.5	11
44	First principle studies of structural, magnetic and elastic properties of orthorhombic rare-earth diaurides intermetallics RAu ₂ (R=La, Ce, Pr and Eu). <i>Materials Chemistry and Physics</i> , 2018, 212, 44-50.	4.0	11
45	Terbium extraction by functionalized surface: experimental and DFT approach. <i>Adsorption</i> , 2020, 26, 117-125.	3.0	11
46	Theoretical studies of CsSnX ₃ (X=Cl, Br and I) for energy storage and hybrid solar cell applications. <i>Materials Today Communications</i> , 2020, 25, 101517.	1.9	11
47	FIXATION OF MICRO OR SUBMICRO AMOUNTS OF Hg(II) IONS ONTO SAWDUST FROM AQUEOUS SOLUTIONS. <i>Main Group Metal Chemistry</i> , 2002, 25, .	1.6	10
48	Adsorption Characteristics of Cr(III) Ions onto Coconut Husk from Aqueous Solution. <i>Adsorption Science and Technology</i> , 2005, 23, 467-478.	3.2	10
49	Electronic structure of the LiA ₂ O ₆ (A=Nb, Ta, and A ²⁺ =W, Mo) ceramics by modified Becke-Johnson potential. <i>Optical Materials</i> , 2016, 58, 466-475.	3.6	10
50	A sensitive non-enzymatic glucose sensor based on MgO entangled nanosheets decorated with CdS nanoparticles: Experimental and DFT study. <i>Journal of Molecular Liquids</i> , 2022, 360, 119366.	4.9	10
51	Functionalized nanospheres for efficient sequestration of cadmium ions. <i>RSC Advances</i> , 2014, 4, 50056-50063.	3.6	9
52	Strongly correlated intermetallic rare-earth monoaurides (Ln-Au): Ab-initio study. <i>Journal of Rare Earths</i> , 2018, 36, 1106-1111.	4.8	9
53	Physical properties and possible applications of gold-based rare earth intermetallics (R-Au): A review. <i>Journal of Magnetism and Magnetic Materials</i> , 2019, 490, 165477.	2.3	9
54	Tuning the Properties of Novel Magnetic Oxide via Co-Bi Co-substitution Including Theoretical Background of Characterization Techniques. <i>Journal of Superconductivity and Novel Magnetism</i> , 2021, 34, 2313-2329.	1.8	9

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55	Selective sensing of NH ₃ and CH ₂ O molecules by novel 2D porous hexagonal boron oxide (B ₃ O ₃) monolayer: A DFT approach. <i>Surfaces and Interfaces</i> , 2022, 29, 101767.	3.0	9
56	Removal of Tm(III) ions from aqueous solution using PAN-incorporated sol-gel matrices. <i>Radiochimica Acta</i> , 2007, 95, 451-457.	1.2	7
57	Complexation of Hg(II) ions with a functionalized adsorbent: A thermodynamic and kinetic approach. <i>Progress in Nuclear Energy</i> , 2018, 105, 146-152.	2.9	7
58	Synthesis and Characterization of Functionalized Nanosilica for Zinc Ion Mitigation; Experimental and Computational Investigations. <i>Molecules</i> , 2020, 25, 5534.	3.8	7
59	Nanotechnology for Water Treatment. <i>Environmental Chemistry for A Sustainable World</i> , 2020, , 143-163.	0.5	7
60	Anodic SnO ₂ Nanoporous Channels Functionalized with CuO Quantum Dots for Selective H ₂ O ₂ Biosensing. <i>ACS Applied Nano Materials</i> , 2022, 5, 9096-9111.	5.0	7
61	Removal of Zn(II) Ions from Aqueous Solution Using BPHA-impregnated Polyurethane Foam. <i>Journal of the Chinese Chemical Society</i> , 2008, 55, 147-154.	1.4	6
62	First-principles studies of pure and fluorine substituted alanines. <i>International Journal of Modern Physics B</i> , 2016, 30, 1650079.	2.0	6
63	A computational study on the characteristics of open-shell H-bonding interaction between carbamic acid (NH ₂ COOH) and HO ₂ , HOS or HSO radicals. <i>Journal of Molecular Modeling</i> , 2019, 25, 189.	1.8	6
64	Al-decorated C ₂₄ N ₂₄ fullerene: A robust single-atom catalyst for CO oxidation. <i>Polyhedron</i> , 2021, , 115497.	2.2	5
65	Theoretical insight of ciprofloxacin removal from water using boron nitride (B ₁₂ N ₁₂) nanocage. <i>Surfaces and Interfaces</i> , 2022, 31, 101982.	3.0	5
66	DFT and post-DFT studies of metallic MXY ₃ -type compounds for low temperature TE applications. <i>Solid State Communications</i> , 2016, 243, 28-35.	1.9	4
67	Equilibrium, kinetic and thermodynamic study of acid yellow-34 adsorption onto <i>Cedrus deodara</i> sawdust. <i>Desalination and Water Treatment</i> , 2016, 57, 18175-18181.	1.0	4
68	Removal of nitrous and carbon mono oxide from flue gases by Si-coordinated nitrogen doped C ₆₀ -fullerene: A DFT approach. <i>Molecular Catalysis</i> , 2021, 509, 111674.	2.0	4
69	Organic-inorganic hybrids: an efficient extractant of environmental mercury ions. <i>Materials Research Express</i> , 2018, 5, 075007.	1.6	3
70	Silicon-doped boron nitride graphyne-like sheet for catalytic N ₂ O reduction: A DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 114, 108186.	2.4	3
71	Sorption Profile of Cd(II) Ions Onto Coconut Husk. <i>Main Group Metal Chemistry</i> , 2003, 26, .	1.6	2
72	Tailored silica nanospheres: an efficient adsorbent for environmental chromium remediation. <i>Radiochimica Acta</i> , 2018, 106, 427-435.	1.2	2

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73	Co Anchored B ₃₆ Cluster as a Novel Single Atom Catalyst for Removing Toxic CO Molecules: A Mechanistic First-Principles Study. <i>ChemistrySelect</i> , 2022, 7, .	1.5	2
74	Controlling Casimir force via coherent driving field. <i>European Physical Journal D</i> , 2016, 70, 1.	1.3	1
75	Depolymerization Study of Pakistani Coal in a Hydrogen Atmosphere. Effect of Operating Conditions. <i>Journal of the Chinese Chemical Society</i> , 2004, 51, 723-727.	1.4	0
76	Molecularly Imprinted Polymeric Nanomaterials for Environmental Analysis. <i>Environmental Chemistry for A Sustainable World</i> , 2019, , 143-168.	0.5	0
77	Synthesis and application of functionalized nano silica for Ag(II) ions sequestration. , 0, 84, 292-298.		0
78	Re-thinking Higher Education Curricula in the Era of Knowledge Economy: A Case Study of Course Codes in the National Curriculum of Pakistan. <i>Sir Syed Journal of Education & Social Research (SJESR)</i> , 2020, 3, 89-96.	0.1	0