Rajeev Ahuja

List of Publications by Citations

952 papers	30,026 citations	79 h-index	130 g-index
987 ext. papers	33,894 ext. citations	4.8 avg, IF	7.55 L-index

#	Paper	IF	Citations
952	Ferromagnetism above room temperature in bulk and transparent thin films of Mn-doped ZnO. *Nature Materials*, **2003**, 2, 673-7	27	1568
951	Calculated elastic properties of M2AlC (M=Ti, V, Cr, Nb and Ta). *Solid State Communications*, **2004**, 129, 589-592	1.6	339
950	Experimental evidence for sub-3-fs charge transfer from an aromatic adsorbate to a semiconductor. *Nature*, **2002**, 418, 620-3	50.4	321
949	Strain Engineering for Phosphorene: The Potential Application as a Photocatalyst. *Journal of Physical Chemistry C*, **2014**, 118, 26560-26568	3.8	314
948	Defect Engineered g-C3N4 for Efficient Visible Light Photocatalytic Hydrogen Production. *Chemistry of Materials*, **2015**, 27, 4930-4933	9.6	308
947	Electronic, bonding, and optical properties of CeO2 and Ce2O3 from first principles. *Physical Review B*, **2001**, 64,	3.3	304
946	Materials science. The hardest known oxide. *Nature*, **2001**, 410, 653-4	50.4	290
945	Phonon related properties of transition metals, their carbides, and nitrides: A first-principles study. *Journal of Applied Physics*, **2007**, 101, 123519	2.5	278
944	Physisorption of nucleobases on graphene: Density-functional calculations. *Physical Review B*, **2007**, 76,	3.3	274
943	Design of High-Efficiency Visible-Light Photocatalysts for Water Splitting: MoS2/AlN(GaN) Heterostructures. *Journal of Physical Chemistry C*, **2014**, 118, 17594-17599	3.8	269
942	Structure of phase change materials for data storage. *Physical Review Letters*, **2006**, 96, 055507	7.4	264
941	Review of two-dimensional materials for photocatalytic water splitting from a theoretical perspective. *Catalysis Science and Technology*, **2017**, 7, 545-559	5.5	251
940	Structural, elastic, and high-pressure properties of cubic TiC, TiN, and TiO. *Physical Review B*, **1996**, 53, 3072-3079	3.3	243
939	Cubic Hf3N4 and Zr3N4: A class of hard materials. *Physical Review B*, **2003**, 68,	3.3	242
938	The importance of strong carbon-metal adhesion for catalytic nucleation of single-walled carbon nanotubes. *Nano Letters*, **2008**, 8, 463-8	11.5	237
937	Hydrogen Storage Materials for Mobile and Stationary Applications: Current State of the Art. *ChemSusChem*, **2015**, 8, 2789-825	8.3	236
936	Single-layer MoS2 as an efficient photocatalyst. *Catalysis Science and Technology*, **2013**, 3, 2214	5.5	236

935	Quasi-Ab initio molecular dynamic study of Fe melting. *Physical Review Letters*, **2000**, 84, 3638-41	7.4	220
934	Li-decorated metal-organic framework 5: a route to achieving a suitable hydrogen storage medium. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 20173-6	11.5	216
933	Mn+1AXn phases in the Ti–Si–C system studied by thin-film synthesis and ab initio calculations. *Physical Review B*, **2004**, 70,	3.3	188
932	Deposition and characterization of ternary thin films within the Ti–Al–C system by DC magnetron sputtering. *Journal of Crystal Growth*, **2006**, 291, 290-300	1.6	187
931	Stability of the body-centred-cubic phase of iron in the Earth's inner core. *Nature*, **2003**, 424, 1032-4	50.4	182
930	Carbon nanomaterials as catalysts for hydrogen uptake and release in NaAlH4. *Nano Letters*, **2009**, 9, 1501-5	11.5	180
929	Structure and bulk modulus of M2AlC (M=Ti, V, and Cr). *Applied Physics Letters*, **2003**, 83, 899-901	3.4	173
928	Magnetism and band gap narrowing in Cu-doped ZnO. *Applied Physics Letters*, **2009**, 94, 142502	3.4	172
927	Bonding and classification of nanolayered ternary carbides. *Physical Review B*, **2004**, 70,	3.3	171
926	Potassium-modified Mg(NH2)2/2 LiH system for hydrogen storage. *Angewandte Chemie - International Edition*, **2009**, 48, 5828-32	16.4	166
925	Electronic structure of nanostructured ZnO from x-ray absorption and emission spectroscopy and the local density approximation. *Physical Review B*, **2004**, 70,	3.3	159
924	Experimental and theoretical identification of a new high-pressure phase of silica. *Nature*, **1997**, 388, 362-365	50.4	158
923	Ferromagnetism in Cu-doped ZnO from first-principles theory. *Physical Review B*, **2006**, 74,	3.3	158
922	Experimental and theoretical identification of a new high-pressure TiO2 polymorph. *Physical Review Letters*, **2001**, 87, 275501	7.4	156
921	Ab initio calculations and experimental determination of the structure of Cr2AlC. *Solid State Communications*, **2004**, 130, 445-449	1.6	154
920	TiO2-based gas sensor: a possible application to SO2. *ACS Applied Materials & Interfaces*, **2013**, 5, 8516-22	9.5	153
919	First-principles study of physisorption of nucleic acid bases on small-diameter carbon nanotubes. *Nanotechnology*, **2008**, 19, 125701	3.4	149
918	Terahertz plasmonics: The rise of toroidal metadevices towards immunobiosensings. *Materials Today*, **2020**, 32, 108-130	21.8	148

917	Rational Design: A High-Throughput Computational Screening and Experimental Validation Methodology for Lead-Free and Emergent Hybrid Perovskites. *ACS Energy Letters*, **2017**, 2, 837-845	20.1	142
916	Symmetry breaking induced bandgap in epitaxial graphene layers on SiC. *Nano Letters*, **2008**, 8, 4464-8	11.5	140
915	Crystal structures of Ti, Zr, and Hf under compression: Theory. *Physical Review B*, **1993**, 48, 16269-16279	3.3	139
914	Transverse conductance of DNA nucleotides in a graphene nanogap from first principles. *Nano Letters*, **2011**, 11, 1941-5	11.5	138
913	Highly Sensitive and Selective Gas Detection Based on Silicene. *Journal of Physical Chemistry C*, **2015**, 119, 16934-16940	3.8	131
912	Elastic and optical properties of □and □Al2O3. *Physical Review B*, **1999**, 59, 12777-12787	3.3	129
911	Optical properties of the group-IVB refractory metal compounds. *Physical Review B*, **1996**, 54, 1673-1681	3.3	124
910	Topological insulating in GeTe/Sb2Te3 phase-change superlattice. *Physical Review Letters*, **2012**, 109, 096802	7.4	117
909	A possible mechanism for the emergence of an additional band gap due to a Ti□□ bond in the TiO2□graphene hybrid system for enhanced photodegradation of methylene blue under visible light. *RSC Advances*, **2014**, 4, 59890-59901	3.7	113
908	Superconductivity in topological insulator Sb2Te3 induced by pressure. *Scientific Reports*, **2013**, 3, 2016	4.9	113
907	Li+ ion conductivity and diffusion mechanism in □Li3N and □Li3N. *Energy and Environmental Science*, **2010**, 3, 1524	35.4	112
906	Electronic and optical properties of RuO2 and IrO2. *Physical Review B*, **2006**, 73,	3.3	110
905	Optical properties of graphite from first-principles calculations. *Physical Review B*, **1997**, 55, 4999-5005	3.3	108
904	Optical properties of Ti3SiC2 and Ti4AlN3. *Applied Physics Letters*, **2008**, 92, 221907	3.4	106
903	Theoretical investigation of the bonding and elastic properties of nanolayered ternary nitrides. *Physical Review B*, **2005**, 71,	3.3	105
902	Crystal structure and elastic-constant anomalies in the magnetic 3d transition metals. *Physical Review B*, **1994**, 50, 5918-5927	3.3	103
901	Borophane as a Benchmate of Graphene: A Potential 2D Material for Anode of Li and Na-Ion Batteries. *ACS Applied Materials & Interfaces*, **2017**, 9, 16148-16158	9.5	101
900	Graphene oxide as a chemically tunable 2-D material for visible-light photocatalyst applications. *Journal of Catalysis*, **2013**, 299, 204-209	7.3	101

899	Metal-nonmetal transition in the boron group elements. *Physical Review Letters*, **2003**, 90, 065701	7.4	101
898	High-pressure structural studies of hematite Fe2O3. *Physical Review B*, **2002**, 65,	3.3	100
897	Quasi ab initio molecular dynamic study of Cu melting. *Physical Review B*, **2000**, 61, 3838-3844	3.3	99
896	Toward the Realization of 2D Borophene Based Gas Sensor. *Journal of Physical Chemistry C*, **2017**, 121, 26869-26876	3.8	98
895	Room temperature ferromagnetism in pristine MgO thin films. *Applied Physics Letters*, **2010**, 96, 232505	3.4	98
894	Structure-based drug designing and immunoinformatics approach for SARS-CoV-2. *Science Advances*, **2020**, 6, eabb8097	14.3	97
893	A high-pressure structure in curium linked to magnetism. *Science*, **2005**, 309, 110-3	33.3	97
892	Structural phase transition of vanadium at 69 GPa. *Physical Review Letters*, **2007**, 98, 085502	7.4	96
891	High-pressure and high-temperature synthesis of the cubic TiO2 polymorph. *Physical Review B*, **2004**, 70,	3.3	96
890	Elasticity of the superconducting metals V, Nb, Ta, Mo, and W at high pressure. *Physical Review B*, **2008**, 77,	3.3	95
889	Pressure-induced reversible amorphization and an amorphous-amorphous transition in Ge□Sb□Te□ phase-change memory material. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 10410-4	11.5	94
888	An ab initio study of the Li-ion battery cathode material Li2FeSiO4. *Electrochemistry Communications*, **2006**, 8, 797-800	5.1	94
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882	Unique melting behavior in phase-change materials for rewritable data storage. *Physical Review Letters*, **2007**, 98, 055505	7.4	84

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876	Relativity and the lead-acid battery. *Physical Review Letters*, **2011**, 106, 018301	7.4	80
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874	Role of catalysts in dehydrogenation of MgH2 nanoclusters. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 8227-31	11.5	79
873	Theoretical investigation of the solubility in (MxM2−x?)AlC (M and M?=Ti,V,Cr). *Physical Review B*, **2003**, 68,	3.3	79
872	A natural shock-induced dense polymorph of rutile with α-PbO2 structure in the suevite from the Ries crater in Germany. *Earth and Planetary Science Letters*, **2001**, 192, 485-495	5.3	76
871	Theoretical and experimental study of the graphite 1s x-ray absorption edges. *Physical Review B*, **1996**, 54, 14396-14404	3.3	76
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869	Theoretical Study of Electronic Transport through DNA Nucleotides in a Double-Functionalized Graphene Nanogap. *Journal of Physical Chemistry C*, **2013**, 117, 15421-15428	3.8	74
868	Theoretical and experimental evidence of enhanced ferromagnetism in Ba and Mn cosubstituted BiFeO3. *Applied Physics Letters*, **2010**, 96, 032903	3.4	74
867	Vacancy-mediated hydrogen desorption in NaAlH4. *Physical Review B*, **2005**, 72,	3.3	74
866	Nanostructured materials for solid-state hydrogen storage: A review of the achievement of COST Action MP1103. *International Journal of Hydrogen Energy*, **2016**, 41, 14404-14428	6.7	74
865	Encapsulating Trogtalite CoSe2 Nanobuds into BCN Nanotubes as High Storage Capacity Sodium Ion Battery Anodes. *Advanced Energy Materials*, **2019**, 9, 1901778	21.8	72
864	General trend for pressurized superconducting hydrogen-dense materials. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 2793-6	11.5	72

863	Rhodium dihydride (RhH2) with high volumetric hydrogen density. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 18618-21	11.5	72
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860	Ab initio calculations of the mechanical properties of Ti3SiC2. *Applied Physics Letters*, **2001**, 79, 1450-1452	3.4	71
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856	The curious case of two dimensional Si2BN: A high-capacity battery anode material. *Nano Energy*, **2017**, 41, 251-260	17.1	68
855	Optical properties of monoclinic SnI2 from relativistic first-principles theory. *Physical Review B*, **1997**, 56, 6851-6861	3.3	68
854	Theoretical confirmation of the high pressure simple cubic phase in calcium. *Physical Review Letters*, **1995**, 75, 3473-3476	7.4	68
853	Role of titanium in hydrogen desorption in crystalline sodium alanate. *Applied Physics Letters*, **2005**, 86, 251913	3.4	67
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851	Theory of the ternary layered system Ti$_2$AlN. *Journal of Applied Physics*, **2002**, 91, 9874	2.5	67
850	Structural and energetic analysis of the hydrogen storage materials LiNH2BH3 and NaNH2BH3 from ab initio calculations. *Physical Review B*, **2009**, 79,	3.3	66
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840	Modelling high-performing batteries with Mxenes: The case of S-functionalized two-dimensional nitride Mxene electrode. *Nano Energy*, **2019**, 58, 877-885	17.1	62
839	Effect of Transition Metal Cations on Stability Enhancement for Molybdate-Based Hybrid Supercapacitor. *ACS Applied Materials & Interfaces*, **2017**, 9, 17977-17991	9.5	61
838	Hybrid density functional study on SrTiO3 for visible light photocatalysis. *International Journal of Hydrogen Energy*, **2012**, 37, 11611-11617	6.7	61
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836	Dynamic atmospheres and winds of cool luminous giants. *Astronomy and Astrophysics*, **2016**, 594, A108	5.1	61
835	Core-shell nanostructures: perspectives towards drug delivery applications. *Journal of Materials Chemistry B*, **2020**,	7.3	61
834	Synthesis, structural and electrochemical properties of sodium nickel phosphate for energy storage devices. *Nanoscale*, **2016**, 8, 11291-305	7.7	61
833	Enhanced DNA Sequencing Performance Through Edge-Hydrogenation of Graphene Electrodes. *Advanced Functional Materials*, **2011**, 21, 2674-2679	15.6	60
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830	Optical properties of Mg-doped VO2: Absorption measurements and hybrid functional calculations. *Applied Physics Letters*, **2012**, 101, 201902	3.4	58
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828	Optical properties of PdO and PtO. *Physical Review B*, **1994**, 50, 2128-2132	3.3	57

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822	Electronic structure of graphite: Effect of hydrostatic pressure. *Physical Review B*, **1995**, 51, 4813-4819	3.3	55
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820	Study of Ti2SC under compression up to 47GPa. *Journal of Alloys and Compounds*, **2008**, 448, L1-L4	5.7	54
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817	The role of Ge2Sb2Te5 in enhancing the performance of functional plasmonic devices. *Materials Today Physics*, **2020**, 12, 100178	8	53
816	Structure of the Ge□Sb□□e phase-change materials studied by theory and experiment. *Solid State Communications*, **2007**, 143, 240-244	1.6	53
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813	Sensing Characteristics of Phosphorene Monolayers toward PH3 and AsH3 Gases upon the Introduction of Vacancy Defects. *Journal of Physical Chemistry C*, **2016**, 120, 20428-20436	3.8	52
812	2D-HfS2 as an efficient photocatalyst for water splitting. *Catalysis Science and Technology*, **2016**, 6, 6605-6614	5.5	52
811	Electronic Structure, Optical Properties, and Photocatalytic Activities of LaFeO3□NaTaO3 Solid Solution. *Journal of Physical Chemistry C*, **2012**, 116, 22767-22773	3.8	52
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800	Toroidal Metaphotonics and Metadevices. *Laser and Photonics Reviews*, **2020**, 14, 1900326	8.3	51
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798	Band gap engineering in BiNbO4 for visible-light photocatalysis. *Applied Physics Letters*, **2012**, 100, 182102	3.4	49
797	Strain induced lithium functionalized graphane as a high capacity hydrogen storage material. *Applied Physics Letters*, **2012**, 101, 103907	3.4	49
796	Tunable Assembly of sp3 Cross-Linked 3D Graphene Monoliths: A First-Principles Prediction. *Advanced Functional Materials*, **2013**, 23, 5846-5853	15.6	49
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787	Graphenylene Monolayers Doped with Alkali or Alkaline Earth Metals: Promising Materials for Clean Energy Storage. *Journal of Physical Chemistry C*, **2017**, 121, 14393-14400	3.8	46
786	Mo- and N-doped BiNbO4 for photocatalysis applications. *Applied Physics Letters*, **2011**, 99, 051909	3.4	46
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