Can Ataca

List of Publications by Year in Descending Order

43 papers	6,247 citations	24 h-index	43 g-index
43 ext. papers	6,915 ext. citations	6.5 avg, IF	6.04 L-index

#	Paper	IF	Citations
43	Intrinsic Ferromagnetism of Two-Dimensional (2D) MnO2 Revisited: A Many-Body Quantum Monte Carlo and DFT+U Study. *Journal of Physical Chemistry C*, **2022**, 126, 5813-5821	3.8	1
42	Stability of adsorption of Mg and Na on sulfur-functionalized MXenes. *Physical Chemistry Chemical Physics*, **2021**, 23, 25424-25433	3.6	2
41	A pathway toward high-throughput quantum Monte Carlo simulations for alloys: A case study of two-dimensional (2D) GaSSe. *Journal of Chemical Physics*, **2021**, 155, 194112	3.9	2
40	Positive and Negative Photoconductivity in Monolayer MoS2 as a Function of Physisorbed Oxygen. *Journal of Physical Chemistry C*, **2021**, 125, 8712-8718	3.8	5
39	Influence of Cr-substitution on the structural, magnetic, electron transport, and mechanical properties of Fe3□r Ge Heusler alloys. *Journal of Magnetism and Magnetic Materials*, **2021**, 521, 167398	2.8	8
38	Comprehensive Study of Lithium Adsorption and Diffusion on Janus Mo/WXY (X, Y = S, Se, Te) Using First-Principles and Machine Learning Approaches. *ACS Applied Materials & Interfaces*, **2021**, 13, 36388-36406	9.5	12
37	Abnormal Phase Transition and Band Renormalization of Guanidinium-Based Organic-Inorganic Hybrid Perovskite. *ACS Applied Materials & Interfaces*, **2021**, 13, 44964-44971	9.5	2
36	Janus PtXnY2□ (X, Y = S, Se, Te; 0□□2) Monolayers for Enhanced Photocatalytic Water Splitting. *Physical Review Applied*, **2020**, 13,	4.3	25
35	Electronic properties of bare and functionalized two-dimensional (2D) tellurene structures. *Physical Chemistry Chemical Physics*, **2020**, 22, 6727-6737	3.6	20
34	Layered Perovskites: Unusual Pressure-Driven Phase Transformation and Band Renormalization in 2D vdW Hybrid Lead Halide Perovskites (Adv. Mater. 12/2020). *Advanced Materials*, **2020**, 32, 2070088	24	
33	Tuneable structure and magnetic properties in Fe3□VxGe alloys. *Journal of Alloys and Compounds*, **2020**, 830, 154403	5.7	9
32	Unusual Pressure-Driven Phase Transformation and Band Renormalization in 2D vdW Hybrid Lead Halide Perovskites. *Advanced Materials*, **2020**, 32, e1907364	24	10
31	Surface Defect Engineering of MoS for Atomic Layer Deposition of TiO Films. *ACS Applied Materials & Interfaces*, **2020**, 12, 48150-48160	9.5	5
30	A first-principles Quantum Monte Carlo study of two-dimensional (2D) GaSe. *Journal of Chemical Physics*, **2020**, 153, 154704	3.9	16
29	Engineering the Electronic, Thermoelectric, and Excitonic Properties of Two-Dimensional Group-III Nitrides through Alloying for Optoelectronic Devices (BAlN, AlGaN, and GaInN). *ACS Applied Materials & Interfaces*, **2020**, 12, 46416-46428	9.5	8
28	Strain effects on electronic and magnetic properties of the monolayer □ RuCl 3: A first-principles and Monte Carlo study. *Journal of Applied Physics*, **2019**, 125, 083903	2.5	20
27	Accurate Predictions of Electron Binding Energies of Dipole-Bound Anions via Quantum Monte Carlo Methods. *Journal of Physical Chemistry Letters*, **2018**, 9, 6185-6190	6.4	16

26	Optical and Electronic Properties of Two-Dimensional Layered Materials. *Nanophotonics*, **2017**, 6, 479-493	6.3	86
25	Torsional Deformations in Subnanometer MoS Interconnecting Wires. *Nano Letters*, **2016**, 16, 1210-7	11.5	27
24	Self-Driven Photodetector and Ambipolar Transistor in Atomically Thin GaTe-MoS2 p-n vdW Heterostructure. *ACS Applied Materials & Interfaces*, **2016**, 8, 2533-9	9.5	126
23	Enhancing light emission efficiency without color change in post-transition metal chalcogenides. *Nanoscale*, **2016**, 8, 5820-5	7.7	10
22	Band Engineering by Controlling vdW Epitaxy Growth Mode in 2D Gallium Chalcogenides. *Advanced Materials*, **2016**, 28, 7375-82	24	23
21	MoS2 Enhanced T-Phase Stabilization and Tunability Through Alloying. *Journal of Physical Chemistry Letters*, **2016**, 7, 2304-9	6.4	48
20	Predicting Electronic Structure in Tricalcium Silicate Phases with Impurities Using First-Principles. *Journal of Physical Chemistry C*, **2015**, 119, 5074-5079	3.8	23
19	Defects activated photoluminescence in two-dimensional semiconductors: interplay between bound, charged, and free excitons. *Scientific Reports*, **2013**, 3, 2657	4.9	726
18	Broad-range modulation of light emission in two-dimensional semiconductors by molecular physisorption gating. *Nano Letters*, **2013**, 13, 2831-6	11.5	566
17	Frictional figures of merit for single layered nanostructures. *Physical Review Letters*, **2012**, 108, 126103	7.4	94
16	Dissociation of H2O at the vacancies of single-layer MoS2. *Physical Review B*, **2012**, 85,	3.3	117
15	Thermally driven crossover from indirect toward direct bandgap in 2D semiconductors: MoSe2 versus MoS2. *Nano Letters*, **2012**, 12, 5576-80	11.5	989
14	Stable, Single-Layer MX2 Transition-Metal Oxides and Dichalcogenides in a Honeycomb-Like Structure. *Journal of Physical Chemistry C*, **2012**, 116, 8983-8999	3.8	992
13	Adsorption of carbon adatoms to graphene and its nanoribbons. *Journal of Applied Physics*, **2011**, 109, 013704	2.5	53
12	Functionalization of Single-Layer MoS2 Honeycomb Structures. *Journal of Physical Chemistry C*, **2011**, 115, 13303-13311	3.8	429
11	A Comparative Study of Lattice Dynamics of Three- and Two-Dimensional MoS2. *Journal of Physical Chemistry C*, **2011**, 115, 16354-16361	3.8	250
10	Mechanical and Electronic Properties of MoS2 Nanoribbons and Their Defects. *Journal of Physical Chemistry C*, **2011**, 115, 3934-3941	3.8	391
9	Perpendicular growth of carbon chains on graphene from first-principles. *Physical Review B*, **2011**, 83,	3.3	43

8	Functionalization of BN honeycomb structure by adsorption and substitution of foreign atoms. *Physical Review B*, **2010**, 82,	3.3	83
7	Effects of silicon and germanium adsorbed on graphene. *Applied Physics Letters*, **2010**, 96, 123112	3.4	55
6	Electronic and magnetic properties of graphane nanoribbons. *Physical Review B*, **2010**, 81,	3.3	122
5	Hydrogen storage of calcium atoms adsorbed on graphene: First-principles plane wave calculations. *Physical Review B*, **2009**, 79,	3.3	277
4	Magnetization of graphane by dehydrogenation. *Applied Physics Letters*, **2009**, 95, 222510	3.4	105
3	Structural, electronic, and magnetic properties of 3d transition metal monatomic chains: First-principles calculations. *Physical Review B*, **2008**, 77,	3.3	61
2	High-capacity hydrogen storage by metallized graphene. *Applied Physics Letters*, **2008**, 93, 043123	3.4	356
1	Atomic and electronic structures of doped silicon nanowires: A first-principles study. *Physical Review B*, **2007**, 76,	3.3	34