Can Ataca

List of Publications by Year
in descending order

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Version: 2024-02-01

43	7,538	186265	254184
papers	citations	28	43
		h-index	g-index

43	43	43	10409
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Intrinsic Ferromagnetism of Two-Dimensional (2D) MnO₂ Revisited: A Many-Body Quantum Monte Carlo and DFT+<i>U</i> Study. Journal of Physical Chemistry C, 2022, 126, 5813-5821.	3.1	6
2	Influence of Cr-substitution on the structural, magnetic, electron transport, and mechanical properties of Fe3â^'Cr Ge Heusler alloys. Journal of Magnetism and Magnetic Materials, 2021, 521, 167398.	2.3	17
3	Positive and Negative Photoconductivity in Monolayer MoS₂ as a Function of Physisorbed Oxygen. Journal of Physical Chemistry C, 2021, 125, 8712-8718.	3.1	19
4	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.	8.0	52
5	Abnormal Phase Transition and Band Renormalization of Guanidinium-Based Organicâ€"Inorganic Hybrid Perovskite. ACS Applied Materials & Interfaces, 2021, 13, 44964-44971.	8.0	8
6	A pathway toward high-throughput quantum Monte Carlo simulations for alloys: A case study of two-dimensional (2D) GaS<i>x</i>Se1â^'<i>x</i>. Journal of Chemical Physics, 2021, 155, 194112.	3.0	7
7	Stability of adsorption of Mg and Na on sulfur-functionalized MXenes. Physical Chemistry Chemical Physics, 2021, 23, 25424-25433.	2.8	8
8	Surface Defect Engineering of MoS2 for Atomic Layer Deposition of TiO2 Films. ACS Applied Materials & Interfaces, 2020, 12, 48150-48160.	8.0	7
9	A first-principles Quantum Monte Carlo study of two-dimensional (2D) GaSe. Journal of Chemical Physics, 2020, 153, 154704.	3.0	23
10	Engineering the Electronic, Thermoelectric, and Excitonic Properties of Two-Dimensional Group-III Nitrides through Alloying for Optoelectronic Devices (B_{1â€"<i>x</i>}Al_{<i>x</i>}N, Al_{1â€"<i>x</i>}Ga_{<i>x</i>}N, and) Tj ETQq0 0 0 rgBT /Ov 46416-46428.	8.0	20
11	Janus <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Pt</mml:mi></mml:math> <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mi>X</mml:mi><mml:mi>n</mml:mi></mml:msub><mml:msub><mml:mi>Y</mml:mi><mml:mrow		

#	Article	IF	Citations
19	Band Engineering by Controlling vdW Epitaxy Growth Mode in 2D Gallium Chalcogenides. Advanced Materials, 2016, 28, 7375-7382.	21.0	28
20	MoS₂ Enhanced T-Phase Stabilization and Tunability Through Alloying. Journal of Physical Chemistry Letters, 2016, 7, 2304-2309.	4.6	54
21	Torsional Deformations in Subnanometer MoS Interconnecting Wires. Nano Letters, 2016, 16, 1210-1217.	9.1	30
22	Self-Driven Photodetector and Ambipolar Transistor in Atomically Thin GaTe-MoS₂ pâ€“n vdW Heterostructure. ACS Applied Materials & Interfaces, 2016, 8, 2533-2539.	8.0	160
23	Enhancing light emission efficiency without color change in post-transition metal chalcogenides. Nanoscale, 2016, 8, 5820-5825.	5.6	13
24	Predicting Electronic Structure in Tricalcium Silicate Phases with Impurities Using First-Principles. Journal of Physical Chemistry C, 2015, 119, 5074-5079.	3.1	38
25	Defects activated photoluminescence in two-dimensional semiconductors: interplay between bound, charged and free excitons. Scientific Reports, 2013, 3, 2657.	3.3	876
26	Broad-Range Modulation of Light Emission in Two-Dimensional Semiconductors by Molecular Physisorption Gating. Nano Letters, 2013, 13, 2831-2836.	9.1	674
27	Frictional Figures of Merit for Single Layered Nanostructures. Physical Review Letters, 2012, 108, 126103.	7.8	110
28	Dissociation of H<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O at the vacancies of single-layer MoS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 85, .	3.2	132
29	Thermally Driven Crossover from Indirect toward Direct Bandgap in 2D Semiconductors: MoSe₂ versus MoS₂. Nano Letters, 2012, 12, 5576-5580.	9.1	1,206
30	Stable, Single-Layer MX₂ Transition-Metal Oxides and Dichalcogenides in a Honeycomb-Like Structure. Journal of Physical Chemistry C, 2012, 116, 8983-8999.	3.1	1,196
31	Perpendicular growth of carbon chains on graphene from first-principles. Physical Review B, 2011, 83, .	3.2	44
32	Adsorption of carbon adatoms to graphene and its nanoribbons. Journal of Applied Physics, 2011, 109, 013704.	2.5	59
33	Functionalization of Single-Layer MoS₂ Honeycomb Structures. Journal of Physical Chemistry C, 2011, 115, 13303-13311.	3.1	484
34	A Comparative Study of Lattice Dynamics of Three- and Two-Dimensional MoS₂. Journal of Physical Chemistry C, 2011, 115, 16354-16361.	3.1	298
35	Mechanical and Electronic Properties of MoS₂ Nanoribbons and Their Defects. Journal of Physical Chemistry C, 2011, 115, 3934-3941.	3.1	427
36	Functionalization of BN honeycomb structure by adsorption and substitution of foreign atoms. Physical Review B, 2010, 82, .	3.2	92

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37	Effects of silicon and germanium adsorbed on graphene. Applied Physics Letters, 2010, 96, .	3.3	63
38	Electronic and magnetic properties of graphane nanoribbons. Physical Review B, 2010, 81, .	3.2	136
39	Hydrogen storage of calcium atoms adsorbed on graphene: First-principles plane wave calculations. Physical Review B, 2009, 79, .	3.2	314
40	Magnetization of graphane by dehydrogenation. Applied Physics Letters, 2009, 95, .	3.3	110
41	Structural, electronic, and magnetic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math>transition metal monatomic chains: First-principles calculations. Physical Review B, 2008, 77, .	3.2	63
42	High-capacity hydrogen storage by metallized graphene. Applied Physics Letters, 2008, 93, .	3.3	397
43	Atomic and electronic structures of doped silicon nanowires: A first-principles study. Physical Review B, 2007, 76, .	3.2	39