A K Singh

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/5847541/publications.pdf

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34	2,999	361413	414414
papers	citations	20	32
		h-index	g-index

35	35	35	4948
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computational Screening of 2D Materials for Photocatalysis. Journal of Physical Chemistry Letters, 2015, 6, 1087-1098.	4.6	641
2	Ab Initio Prediction of Piezoelectricity in Two-Dimensional Materials. ACS Nano, 2015, 9, 9885-9891.	14.6	445
3	Computational discovery of single-layer III-V materials. Physical Review B, 2013, 87, .	3.2	318
4	Computational prediction of two-dimensional group-IV mono-chalcogenides. Applied Physics Letters, 2014, 105, .	3.3	245
5	van der Waals Epitaxial Growth of Graphene on Sapphire by Chemical Vapor Deposition without a Metal Catalyst. ACS Nano, 2013, 7, 385-395.	14.6	211
6	Electrochemical Stability of Metastable Materials. Chemistry of Materials, 2017, 29, 10159-10167.	6.7	168
7	Characterization of Few-Layer 1Tâ€² MoTe₂ by Polarization-Resolved Second Harmonic Generation and Raman Scattering. ACS Nano, 2016, 10, 9626-9636.	14.6	148
8	Ab initiosynthesis of single-layer III-V materials. Physical Review B, 2014, 89, .	3.2	112
9	Rutile Alloys in the Mnâ€“Sbâ€“O System Stabilize Mn³⁺ To Enable Oxygen Evolution in Strong Acid. ACS Catalysis, 2018, 8, 10938-10948.	11.2	97
10	MPInterfaces: A Materials Project based Python tool for high-throughput computational screening of interfacial systems. Computational Materials Science, 2016, 122, 183-190.	3.0	95
11	The structural phases and vibrational properties of Mo _{1â^'x} W _x Te ₂ alloys. 2D Materials, 2017, 4, 045008.	4.4	65
12	Doping-controlled phase transitions in single-layer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> Physical Review B, 2017, 96, .	3.2	62
13	Computational methods for 2D materials: discovery, property characterization, and application design. Journal of Physics Condensed Matter, 2017, 29, 473001.	1.8	55
14	Analyzing Feâ€“Zn system using molecular dynamics, evolutionary neural nets and multi-objective genetic algorithms. Computational Materials Science, 2009, 46, 821-827.	3.0	42
15	Discovery of Manganese-Based Solar Fuel Photoanodes via Integration of Electronic Structure Calculations, Pourbaix Stability Modeling, and High-Throughput Experiments. ACS Energy Letters, 2017, 2, 2307-2312.	17.4	36
16	Inâ€situpatterned laser deposition of highâ€TcYâ€Baâ€Cuâ€O superconducting thin films. Journal of Applied Physics, 1990, 67, 3448-3451.	2.5	32
17	An Antimony Selenide Molecular Ink for Flexible Broadband Photodetectors. Advanced Electronic Materials, 2016, 2, 1600182.	5.1	31
18	Al2O3 as a suitable substrate and a dielectric layer for n-layer MoS2. Applied Physics Letters, 2015, 107, 053106.	3.3	30

#	Article	IF	Citations
19	Identification and Optimization of AB₂Phases Using Principal Component Analysis, Evolutionary Neural Nets, and Multiobjective Genetic Algorithms. Materials and Manufacturing Processes, 2009, 24, 274-281.	4.7	25
20	Genetic algorithm prediction of two-dimensional group-IV dioxides for dielectrics. Physical Review B, 2017, 95, .	3.2	23
21	Surface chemistry and structure of silicon oxycarbide gels and glasses. Journal of Sol-Gel Science and Technology, 1997, 8, 371-376.	2.4	20
22	Two-dimensional forms of robust CO2 reduction photocatalysts. Npj 2D Materials and Applications, 2020, 4, .	7.9	20
23	Exfoliation of boron carbide into ultrathin nanosheets. Nanoscale, 2021, 13, 1652-1662.	5.6	16
24	Excitonic effects in absorption spectra of carbon dioxide reduction photocatalysts. Npj Computational Materials, 2021, 7, .	8.7	12
25	Hot Rolling of a Non-heat Treatable Aluminum Alloy: Thermo-Mechanical and Microstructure Evolution Model. Transactions of the Indian Institute of Metals, 2017, 70, 1387-1398.	1.5	10
26	Insitufabrication of epitaxial YBa2Cu3O7films on latticeâ€mismatched (100) YSâ€ZrO2substrates by the pulsed laser evaporation method. Journal of Applied Physics, 1990, 67, 3452-3455.	2.5	9
27	The Nanocrystal Superlattice Pressure Cell: A Novel Approach To Study Molecular Bundles under Uniaxial Compression. Nano Letters, 2014, 14, 4763-4766.	9.1	9
28	Atom Probe Tomography Analysis of Ag Doping in 2D Layered Material (PbSe)₅(Bi₂Se₃)₃. Nano Letters, 2016, 16, 6064-6069.	9.1	8
29	Computational synthesis of 2D materials: A high-throughput approach to materials design. Computational Materials Science, 2022, 207, 111238.	3.0	7
30	Prediction of entropy stabilized incommensurate phases in the system MoS2â^'MoTe2. Journal of Applied Physics, 2016, 120, 155101.	2.5	4
31	Synthesis of Sic Clusters in a Nonthermal Microwave Plasma. Materials Research Society Symposia Proceedings, 1990, 206, 551.	0.1	1
32	In-Situ Processing of Epitaxial and Textured High Tc Superconducting Hoba2Cu3O7.X Thin Films By Pulsed Laser Evaporation Technique. Materials Research Society Symposia Proceedings, 1989, 169, 459.	0.1	0
33	Inâ€Situ Fabrication of YBa2Cu3O7â€x Superconducting Thin Films Directly on Silicon Substrates with Tc0 > 77K. Materials Research Society Symposia Proceedings, 1989, 169, 481.	0.1	0
34	Laser-Assisted Surface Modification of 4340 Steel with Iron-Aluminum Alloys. Materials Research Society Symposia Proceedings, 2002, 750, 1.	0.1	0