

A K Singh

List of Publications by Year in descending order

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34
papers

2,999
citations

361413

20
h-index

414414

32
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35
all docs

35
docs citations

35
times ranked

4948
citing authors

#	ARTICLE	IF	CITATIONS
1	Computational synthesis of 2D materials: A high-throughput approach to materials design. Computational Materials Science, 2022, 207, 111238.	3.0	7
2	Exfoliation of boron carbide into ultrathin nanosheets. Nanoscale, 2021, 13, 1652-1662.	5.6	16
3	Excitonic effects in absorption spectra of carbon dioxide reduction photocatalysts. Npj Computational Materials, 2021, 7, .	8.7	12
4	Two-dimensional forms of robust CO ₂ reduction photocatalysts. Npj 2D Materials and Applications, 2020, 4, .	7.9	20
5	Rutile Alloys in the Mn–Sb–O System Stabilize Mn ³⁺ To Enable Oxygen Evolution in Strong Acid. ACS Catalysis, 2018, 8, 10938-10948.	11.2	97
6	Doping-controlled phase transitions in single-layer MoS_2 . Physical Review B, 2017, 96, .	10.2	103
7	Electrochemical Stability of Metastable Materials. Chemistry of Materials, 2017, 29, 10159-10167.	6.7	168
8	The structural phases and vibrational properties of Mo_2WTe_2 alloys. 2D Materials, 2017, 4, 045008.	4.4	65
9	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
10	Computational methods for 2D materials: discovery, property characterization, and application design. Journal of Physics Condensed Matter, 2017, 29, 473001.	1.8	55
11	Genetic algorithm prediction of two-dimensional group-IV dioxides for dielectrics. Physical Review B, 2017, 95, .	3.2	23
12	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
13	Prediction of entropy stabilized incommensurate phases in the system $\text{MoS}_2/\text{MoTe}_2$. Journal of Applied Physics, 2016, 120, 155101.	2.5	4
14	Atom Probe Tomography Analysis of Ag Doping in 2D Layered Material $(\text{PbSe})_5(\text{Bi}_2\text{Se}_3)_3$. Nano Letters, 2016, 16, 6064-6069.	9.1	8
15	Characterization of Few-Layer $\text{1T}'\text{MoTe}_2$ by Polarization-Resolved Second Harmonic Generation and Raman Scattering. ACS Nano, 2016, 10, 9626-9636.	14.6	148
16	An Antimony Selenide Molecular Ink for Flexible Broadband Photodetectors. Advanced Electronic Materials, 2016, 2, 1600182.	5.1	31
17	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
18	Computational Screening of 2D Materials for Photocatalysis. Journal of Physical Chemistry Letters, 2015, 6, 1087-1098.	4.6	641

#	ARTICLE	IF	CITATIONS
19	Al ₂ O ₃ as a suitable substrate and a dielectric layer for n-layer MoS ₂ . Applied Physics Letters, 2015, 107, 053106.	3.3	30
20	<i>Ab Initio</i> Prediction of Piezoelectricity in Two-Dimensional Materials. ACS Nano, 2015, 9, 9885-9891.	14.6	445
21	Computational prediction of two-dimensional group-IV mono-chalcogenides. Applied Physics Letters, 2014, 105, .	3.3	245
22	<i>Ab initio</i> synthesis of single-layer III-V materials. Physical Review B, 2014, 89, .	3.2	112
23	The Nanocrystal Superlattice Pressure Cell: A Novel Approach To Study Molecular Bundles under Uniaxial Compression. Nano Letters, 2014, 14, 4763-4766.	9.1	9
24	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
25	Computational discovery of single-layer III-V materials. Physical Review B, 2013, 87, .	3.2	318
26	Identification and Optimization of AB ₂ Phases Using Principal Component Analysis, Evolutionary Neural Nets, and Multiobjective Genetic Algorithms. Materials and Manufacturing Processes, 2009, 24, 274-281.	4.7	25
27	Analyzing Fe-Zn system using molecular dynamics, evolutionary neural nets and multi-objective genetic algorithms. Computational Materials Science, 2009, 46, 821-827.	3.0	42
28	Laser-Assisted Surface Modification of 4340 Steel with Iron-Aluminum Alloys. Materials Research Society Symposia Proceedings, 2002, 750, 1.	0.1	0
29	Surface chemistry and structure of silicon oxycarbide gels and glasses. Journal of Sol-Gel Science and Technology, 1997, 8, 371-376.	2.4	20
30	Synthesis of SiC Clusters in a Nonthermal Microwave Plasma. Materials Research Society Symposia Proceedings, 1990, 206, 551.	0.1	1
31	In-situ patterned laser deposition of high-T _c YBaCuO superconducting thin films. Journal of Applied Physics, 1990, 67, 3448-3451.	2.5	32
32	In-situ fabrication of epitaxial YBa ₂ Cu ₃ O ₇ films on lattice-mismatched (100) Y ₂ ZrO ₂ substrates by the pulsed laser evaporation method. Journal of Applied Physics, 1990, 67, 3452-3455.	2.5	9
33	In-Situ Processing of Epitaxial and Textured High T _c Superconducting YBa ₂ Cu ₃ O _{7-x} Thin Films By Pulsed Laser Evaporation Technique. Materials Research Society Symposia Proceedings, 1989, 169, 459.	0.1	0
34	In-situ Fabrication of YBa ₂ Cu ₃ O _{7-x} Superconducting Thin Films Directly on Silicon Substrates with T _c > 77K. Materials Research Society Symposia Proceedings, 1989, 169, 481.	0.1	0