Alexander G Kvashnin

List of Publications by Year
in descending order

		201674	95266
69	4,845	27	68
papers	citations	h-index	g-index
69	69	69	6536
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Diamane quasicrystals. Applied Surface Science, 2022, 572, 151362.	6.1	16
2	Nanohardness from First Principles with Active Learning on Atomic Environments. Journal of Chemical Theory and Computation, 2022, 18, 1109-1121.	5.3	10
3	Computational Design of Gas Sensors Based on V3S4 Monolayer. Nanomaterials, 2022, 12, 774.	4.1	7
4	Srâ€Doped Superionic Hydrogen Glass: Synthesis and Properties of SrH₂₂. Advanced Materials, 2022, 34, e2200924.	21.0	10
5	Efficient Synthesis of WB_{5â€“<i>x</i>}â€“WB₂ Powders with Selectivity for WB_{5â€“<i>x</i>} Content. Inorganic Chemistry, 2022, 61, 6773-6784.	4.0	3
6	GIPAW Pseudopotentials of d Elements for Solid-State NMR. Materials, 2022, 15, 3347.	2.9	4
7	Map of Two-Dimensional Tungsten Chalcogenide Compounds (Wâ€“S, Wâ€“Se, Wâ€“Te) Based on USPEX Evolutionary Search. JETP Letters, 2022, 115, 292-296.	1.4	3
8	Largeâ€Scale Synthesis and Applications of Hafniumâ€“Tantalum Carbides. Advanced Functional Materials, 2022, 32, .	14.9	8
9	Crystal Structure Evolution of Fluorine under High Pressure. Journal of Physical Chemistry C, 2022, 126, 11358-11364.	3.1	5
10	Novel Strongly Correlated Europium Superhydrides. Journal of Physical Chemistry Letters, 2021, 12, 32-40.	4.6	33
11	Synthesis of molecular metallic barium superhydride: pseudocubic BaH12. Nature Communications, 2021, 12, 273.	12.8	66
12	Anomalous Highâ€Temperature Superconductivity in YH₆. Advanced Materials, 2021, 33, e2006832.	21.0	196
13	Computational Modeling of 2D Materials under High Pressure and Their Chemical Bonding: Silicene as Possible Field-Effect Transistor. ACS Nano, 2021, 15, 6861-6871.	14.6	18
14	Superconductivity at 253â€¯K in lanthanumâ€“yttrium ternary hydrides. Materials Today, 2021, 48, 18-28.	14.2	119
15	Novel two-dimensional boron oxynitride predicted using the USPEX evolutionary algorithm. Physical Chemistry Chemical Physics, 2021, 23, 26178-26184.	2.8	4
16	Superconductivity at 161â€¯K in thorium hydride ThH10: Synthesis and properties. Materials Today, 2020, 33, 36-44.	14.2	187
17	Computational Search for New Wâ€“Moâ€“B Compounds. Chemistry of Materials, 2020, 32, 7028-7035.	6.7	22
18	Environmentally Friendly Method of Silicon Recycling: Synthesis of Silica Nanoparticles in an Aqueous Solution. ACS Sustainable Chemistry and Engineering, 2020, 8, 14006-14012.	6.7	9

#	Article	IF	Citations
19	The Volumetric Source Function: Looking Inside van der Waals Interactions. Scientific Reports, 2020, 10, 7816.	3.3	10
20	Phase Transitions in Tungsten Monoborides. JETP Letters, 2020, 111, 343-349.	1.4	3
21	Structure, Stability, and Mechanical Properties of Boron-Rich Moâ€“B Phases: A Computational Study. Journal of Physical Chemistry Letters, 2020, 11, 2393-2401.	4.6	30
22	WB 5âˆ’ x : Synthesis, Properties, and Crystal Structureâ€"New Insights into the Longâ€Debated Compound. Advanced Science, 2020, 7, 2000775.	11.2	17
23	Youngâ€™s Modulus and Tensile Strength of Ti₃C₂ MXene Nanosheets As Revealed by <i>In Situ</i> TEM Probing, AFM Nanomechanical Mapping, and Theoretical Calculations. Nano Letters, 2020, 20, 5900-5908.	9.1	88
24	Superconductivity of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaH</mml:mi><mml:mn>10</mml:mn></mml:msub></m and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaH</mml:mi><mml:mn>16</mml:mn></mml:msub></m polyhydrides. Physical Review B, 2020, 101, .	3.2	62
25	High-Pressure Synthesis of Magnetic Neodymium Polyhydrides. Journal of the American Chemical Society, 2020, 142, 2803-2811.	13.7	59
26	Exotic Two-Dimensional Structure: The First Case of Hexagonal NaCl. Journal of Physical Chemistry Letters, 2020, 11, 3821-3827.	4.6	38
27	On Distribution of Superconductivity in Metal Hydrides. Current Opinion in Solid State and Materials Science, 2020, 24, 100808.	11.5	104
28	Mechanical Engineering Effect in Electronic and Optical Properties of Graphene Nanomeshes. ACS Applied Materials & Interfaces, 2020, 12, 55189-55194.	8.0	9
29	Computational discovery of hard and superhard materials. Journal of Applied Physics, 2019, 126, .	2.5	46
30	Nonstoichiometric Phases of Two-Dimensional Transition-Metal Dichalcogenides: From Chalcogen Vacancies to Pure Metal Membranes. Journal of Physical Chemistry Letters, 2019, 10, 6492-6498.	4.6	15
31	Novel Unexpected Reconstructions of (100) and (111) Surfaces of NaCl: Theoretical Prediction. Scientific Reports, 2019, 9, 14267.	3.3	21
32	Stability and magnetism of FeN high-pressure phases. Physical Chemistry Chemical Physics, 2019, 21, 5262-5273.	2.8	12
33	Stable and hard hafnium borides: A first-principles study. Journal of Applied Physics, 2019, 125, .	2.5	13
34	Two-Dimensional CuO Inside the Supportive Bilayer Graphene Matrix. Journal of Physical Chemistry C, 2019, 123, 17459-17465.	3.1	12
35	Iron Superhydrides FeH₅ and FeH₆: Stability, Electronic Properties, and Superconductivity. Journal of Physical Chemistry C, 2018, 122, 4731-4736.	3.1	48
36	Actinium Hydrides AcH₁₀, AcH₁₂, and AcH₁₆ as High-Temperature Conventional Superconductors. Journal of Physical Chemistry Letters, 2018, 9, 1920-1926.	4.6	100

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37	Layered heterostructures based on graphene, hexagonal zinc oxide and molybdenum disulfide: Modeling of geometry and electronic properties. Computational Materials Science, 2018, 142, 32-37.	3.0	7
38	High-Temperature Superconductivity in a Thâ€"H System under Pressure Conditions. ACS Applied Materials & Interfaces, 2018, 10, 43809-43816.	8.0	95
39	Uranium polyhydrides at moderate pressures: Prediction, synthesis, and expected superconductivity. Science Advances, 2018, 4, eaat9776.	10.3	82
40	New Tungsten Borides, Their Stability and Outstanding Mechanical Properties. Journal of Physical Chemistry Letters, 2018, 9, 3470-3477.	4.6	61
41	Computational Materials Discovery: Dream or Reality?. , 2018, , 1-14.		3
42	Computational Search for Novel Hard Chromium-Based Materials. Journal of Physical Chemistry Letters, 2017, 8, 755-764.	4.6	62
43	Fullerite-based nanocomposites with ultrahigh stiffness. Theoretical investigation. Carbon, 2017, 115, 546-549.	10.3	15
44	Novel hybrid C/BN two-dimensional heterostructures. Nanotechnology, 2017, 28, 085205.	2.6	8
45	Estimation of graphene surface stability against the adsorption of environmental and technological chemical agents. Physica Status Solidi (B): Basic Research, 2017, 254, 1600702.	1.5	5
46	New allotropic forms of carbon based on Đ¡60 and Đ¡20 fullerenes with specific mechanical characteristics. JETP Letters, 2017, 105, 419-425.	1.4	3
47	Stable reconstruction of the (110) surface and its role in pseudocapacitance of rutile-like RuO2. Scientific Reports, 2017, 7, 10357.	3.3	30
48	Features of Electronic, Mechanical, and Electromechanical Properties of Fluorinated Diamond Films of Nanometer Thickness. Journal of Physical Chemistry C, 2017, 121, 28484-28489.	3.1	29
49	The possible formation of a magnetic FeS2 phase in the two-dimensional MoS2 matrix. Physical Chemistry Chemical Physics, 2016, 18, 26956-26959.	2.8	1
50	Heterostructures based on graphene and MoS2layers decorated by C60fullerenes. Nanotechnology, 2016, 27, 365201.	2.6	11
51	Ionic Graphitization of Ultrathin Films of Ionic Compounds. Journal of Physical Chemistry Letters, 2016, 7, 2659-2663.	4.6	9
52	Toward the Ultra-incompressible Carbon Materials. Computational Simulation and Experimental Observation. Journal of Physical Chemistry Letters, 2015, 6, 2147-2152.	4.6	16
53	Flexoelectricity in Carbon Nanostructures: Nanotubes, Fullerenes, and Nanocones. Journal of Physical Chemistry Letters, 2015, 6, 2740-2744.	4.6	68
54	Hydrogen adsorption study. Formation of quantum dots on graphene nanoribbons within tight-binding approach. Nanotechnology, 2015, 26, 175704.	2.6	1

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55	Transport investigation of branched graphene nanoflakes. Nanotechnology, 2015, 26, 385705.	2.6	7
56	Radiation-Induced Nucleation of Diamond from Amorphous Carbon: Effect of Hydrogen. Journal of Physical Chemistry Letters, 2014, 5, 1924-1928.	4.6	26
57	Phase Diagram of Quasi-Two-Dimensional Carbon, From Graphene to Diamond. Nano Letters, 2014, 14, 676-681.	9.1	154
58	Lonsdaleite Films with Nanometer Thickness. Journal of Physical Chemistry Letters, 2014, 5, 541-548.	4.6	56
59	Spontaneous Graphitization of Ultrathin Cubic Structures: A Computational Study. Nano Letters, 2014, 14, 7126-7130.	9.1	31
60	Graphitic Phase of NaCl. Bulk Properties and Nanoscale Stability. Journal of Physical Chemistry Letters, 2014, 5, 4014-4019.	4.6	16
61	Investigation of new superhard carbon allotropes with promising electronic properties. Journal of Applied Physics, 2013, 114, 183708.	2.5	10
62	Strong Influence of Graphane Island Configurations on the Electronic Properties of a Mixed Graphene/Graphane Superlattice. Journal of Physical Chemistry C, 2012, 116, 20035-20039.	3.1	13
63	Influence of Size Effect on the Electronic and Elastic Properties of Diamond Films with Nanometer Thickness. Journal of Physical Chemistry C, 2011, 115, 132-136.	3.1	82
64	Theoretical Study of Elastic Properties of SiC Nanowires of Different Shapes. Journal of Nanoscience and Nanotechnology, 2010, 10, 4992-4997.	0.9	3
65	Large Scale Growth and Characterization of Atomic Hexagonal Boron Nitride Layers. Nano Letters, 2010, 10, 3209-3215.	9.1	2,317
66	Theoretical Study of Atomic Structure and Elastic Properties of Branched Silicon Nanowires. ACS Nano, 2010, 4, 2784-2790.	14.6	4
67	The Theoretical Study of Mechanical Properties of Graphene Membranes. Fullerenes Nanotubes and Carbon Nanostructures, 2010, 18, 497-500.	2.1	17
68	Diamond-like C2H nanolayer, diamane: Simulation of the structure and properties. JETP Letters, 2009, 90, 134-138.	1.4	169
69	Density functional study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:mo>âŸ¨</mml:mo><mml:mrow><mml:mn>110</mml:mn></mml:mrow><mml:mo>âŸ thin silicon nanowires. Physical Review B, 2008, 77, .	3.2	27