

Andrey A Kistanov

List of Publications by Year in descending order

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51
papers

1,121
citations

394421

19
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414414

32
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all docs

51
docs citations

51
times ranked

1207
citing authors

#	ARTICLE	IF	CITATIONS
1	Discerning phase-matrices for individual nitride inclusions within ultra-high-strength steel: experiment driven DFT investigation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1456-1461.	2.8	3
2	Exploring Mechanisms of Hydration and Carbonation of MgO and Mg(OH) ₂ in Reactive Magnesium Oxide-Based Cements. <i>Journal of Physical Chemistry C</i> , 2022, 126, 6196-6206.	3.1	18
3	Family of Two-Dimensional Transition Metal Dichlorides: Fundamental Properties, Structural Defects, and Environmental Stability. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 2165-2172.	4.6	19
4	Nickel nanoparticle-activated MoS ₂ for efficient visible light photocatalytic hydrogen evolution. <i>Nanoscale</i> , 2022, 14, 8601-8610.	5.6	11
5	Theoretical aspects of sulfide and selenides: Structure, point defects, and electronic structure modifications. , 2022, , 57-79.		0
6	Incorporation of Si atoms into CrCoNiFe high-entropy alloy: a DFT study. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 135703.	1.8	5
7	First-Principles Prediction of Two-Dimensional B ₃ C ₂ P ₃ and B ₂ C ₄ P ₂ : Structural Stability, Fundamental Properties, and Renewable Energy Applications. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 3436-3442.	4.6	34
8	Vacancy-Induced Niobate Perovskite-Tungsten Bronze Composite for Synergetic Tuning of Ferroelectricity and Band Gaps. <i>Journal of Physical Chemistry C</i> , 2021, 125, 8890-8898.	3.1	8
9	Unveiling interactions of non-metallic inclusions within advanced ultra-high-strength steel: A spectro-microscopic determination and first-principles elucidation. <i>Scripta Materialia</i> , 2021, 197, 113791.	5.2	8
10	Point Defects in Two-Dimensional \hat{I}^3 -Phosphorus Carbide. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 620-626.	4.6	21
11	In-situ quantification and density functional theory elucidation of phase transformation in carbon steel during quenching and partitioning. <i>Acta Materialia</i> , 2021, 221, 117361.	7.9	12
12	Synthesis and Characterization of the Ternary Nitride Semiconductor Zn ₂ VN ₃ : Theoretical Prediction, Combinatorial Screening, and Epitaxial Stabilization. <i>Chemistry of Materials</i> , 2021, 33, 9306-9316.	6.7	12
13	Impact of various dopant elements on the electronic structure of Cu ₂ ZnSnS ₄ (CZTS) thin films: a DFT study. <i>CrystEngComm</i> , 2020, 22, 5786-5791.	2.6	8
14	The interaction of two-dimensional \hat{I}^{\pm} - and \hat{I}^2 -phosphorus carbide with environmental molecules: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 11307-11313.	2.8	6
15	The first-principles study of the adsorption of NH ₃ , NO, and NO ₂ gas molecules on InSe-like phosphorus carbide. <i>New Journal of Chemistry</i> , 2020, 44, 9377-9381.	2.8	9
16	Two-Dimensional Black Phosphorus Carbide: Rippling and Formation of Nanotubes. <i>Journal of Physical Chemistry C</i> , 2020, 124, 10235-10243.	3.1	32
17	Adsorption of Common Transition Metal Atoms on Arsenene: A First-Principles Study. <i>Russian Journal of Physical Chemistry A</i> , 2019, 93, 1088-1092.	0.6	3
18	Environmental stability of bismuthene: oxidation mechanism and structural stability of 2D pnictogens. <i>Journal of Materials Chemistry C</i> , 2019, 7, 9195-9202.	5.5	40

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19	First-Principles Study of Interaction of Bismuthene with Small Gas Molecules. ChemistrySelect, 2019, 4, 10928-10933.	1.5	12
20	Ultrafast diffusive cross-sheet motion of lithium through antimonene with 2 + 1 dimensional kinetics. Journal of Materials Chemistry A, 2019, 7, 2901-2907.	10.3	19
21	Effect of oxygen doping on the stability and band structure of borophene nanoribbons. Chemical Physics Letters, 2019, 728, 53-56.	2.6	32
22	A First-Principles Study on the Adsorption of Small Molecules on Arsenene: Comparison of Oxidation Kinetics in Arsenene, Antimonene, Phosphorene, and InSe. ChemPhysChem, 2019, 20, 575-580.	2.1	42
23	Effects of graphene/BN encapsulation, surface functionalization and molecular adsorption on the electronic properties of layered InSe: a first-principles study. Physical Chemistry Chemical Physics, 2018, 20, 12939-12947.	2.8	27
24	Electronic structure of graphene and BN-supported phosphorene. Physica B: Condensed Matter, 2018, 534, 63-67.	2.7	36
25	A first-principles study on the adsorption of small molecules on antimonene: oxidation tendency and stability. Journal of Materials Chemistry C, 2018, 6, 4308-4317.	5.5	68
26	Exploring the charge localization and band gap opening of borophene: a first-principles study. Nanoscale, 2018, 10, 1403-1410.	5.6	77
27	Atomic-scale mechanisms of defect- and light-induced oxidation and degradation of InSe. Journal of Materials Chemistry C, 2018, 6, 518-525.	5.5	43
28	Strain engineering of antimonene by a first-principles study: Mechanical and electronic properties. Physical Review B, 2018, 98, .	3.2	82
29	Effects of substrate and environmental adsorbates on the electronic properties and structural stability of antimonene. Journal of Materials Science, 2018, 53, 15559-15568.	3.7	11
30	Bending instability of few-layer graphene embedded in strained polymer matrix. Letters on Materials, 2018, 8, 278-281.	0.7	2
31	Strain and water effects on the electronic structure and chemical activity of in-plane graphene/silicene heterostructure. Journal of Physics Condensed Matter, 2017, 29, 095302.	1.8	25
32	Breathing subsonic crowdion in Morse lattices. Computational Condensed Matter, 2017, 13, 59-64.	2.1	34
33	The role of H ₂ O and O ₂ molecules and phosphorus vacancies in the structure instability of phosphorene. 2D Materials, 2017, 4, 015010.	4.4	101
34	Strain and defects engineering of phosphorene. , 2017, , .		1
35	Simulation of energy transport in crystal with NaCl structure assisted by discrete breathers. Letters on Materials, 2017, 7, 77-80.	0.7	1
36	Large Electronic Anisotropy and Enhanced Chemical Activity of Highly Rippled Phosphorene. Journal of Physical Chemistry C, 2016, 120, 6876-6884.	3.1	68

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37	The reason for existence of discrete breathers in 2D and 3D Morse crystals. Letters on Materials, 2016, 6, 221-226.	0.7	5
38	Numerical modeling of 3D discrete breathers in fcc Ni. Letters on Materials, 2016, 6, 304-308.	0.7	4
39	Moving discrete breathers in bcc metals V, Fe and W. Computational Materials Science, 2015, 98, 88-92.	3.0	43
40	Properties of moving discrete breathers in a monoatomic two-dimensional crystal. Journal of Experimental and Theoretical Physics, 2014, 119, 766-771.	0.9	13
41	Effect of small perturbations on the evolution of polycrystalline structure during plastic deformation. Physics of Metals and Metallography, 2014, 115, 918-925.	1.0	2
42	Interaction of propagating discrete breathers with a vacancy in a two-dimensional crystal. Technical Physics Letters, 2014, 40, 657-661.	0.7	19
43	Moving discrete breathers in a monoatomic two-dimensional crystal. JETP Letters, 2014, 99, 353-357.	1.4	42
44	Properties of discrete breathers in 2D and 3D Morse crystals. Letters on Materials, 2014, 4, 315-318.	0.7	6
45	Discrete breathers in crystals with the NaCl structure. Russian Physics Journal, 2013, 56, 180-191.	0.4	10
46	Energy exchange between discrete breathers in crystal with NaCl structure. Technical Physics Letters, 2013, 39, 618-620.	0.7	15
47	Spontaneous excitation of discrete breathers in crystals with the NaCl structure at elevated temperatures. Physics of the Solid State, 2012, 54, 1648-1651.	0.6	12
48	A molecular dynamics study of [111]-polarized gap discrete breathers in a crystal with NaCl-type structure. Technical Physics Letters, 2012, 38, 676-679.	0.7	17
49	The equilibrium states of $A_{1-x}B_x$ binary alloys in the hard-sphere and pair-binding model. Russian Physics Journal, 2012, 54, 1128-1136.	0.4	1
50	Temperature dependence of high-energy atoms density in the crystal with NaCl structure. Letters on Materials, 2012, 2, 143-146.	0.7	2
51	Unveiling Interactions of Non-Metallic Inclusions within Advanced Ultra-High Strength Steel: A Spectro-Microscopic Determination and First-Principles Elucidation. SSRN Electronic Journal, 0, , .	0.4	0