Andrey A Kistanov

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	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
2	Strain engineering of antimonene by a first-principles study: Mechanical and electronic properties. Physical Review B, 2018, 98, .	3.2	82
3	Exploring the charge localization and band gap opening of borophene: a first-principles study. Nanoscale, 2018, 10, 1403-1410.	5.6	77
4	Large Electronic Anisotropy and Enhanced Chemical Activity of Highly Rippled Phosphorene. Journal of Physical Chemistry C, 2016, 120, 6876-6884.	3.1	68
5	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
6	Moving discrete breathers in bcc metals V, Fe and W. Computational Materials Science, 2015, 98, 88-92.	3.0	43
7	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
8	Moving discrete breathers in a monoatomic two-dimensional crystal. JETP Letters, 2014, 99, 353-357.	1.4	42
9	A Firstâ€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
10	Environmental stability of bismuthene: oxidation mechanism and structural stability of 2D pnictogens. Journal of Materials Chemistry C, 2019, 7, 9195-9202.	5.5	40
11	Electronic structure of graphene– and BN–supported phosphorene. Physica B: Condensed Matter, 2018, 534, 63-67.	2.7	36
12	Breathing subsonic crowdion in Morse lattices. Computational Condensed Matter, 2017, 13, 59-64.	2.1	34
13	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. Journal of Physical Chemistry Letters, 2021, 12, 3436-3442.	4.6	34
14	Effect of oxygen doping on the stability and band structure of borophene nanoribbons. Chemical Physics Letters, 2019, 728, 53-56.	2.6	32
15	Two-Dimensional Black Phosphorus Carbide: Rippling and Formation of Nanotubes. Journal of Physical Chemistry C, 2020, 124, 10235-10243.	3.1	32
16	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
17	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
18	Point Defects in Two-Dimensional γ-Phosphorus Carbide. Journal of Physical Chemistry Letters, 2021, 12, 620-626.	4.6	21

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19	Interaction of propagating discrete breathers with a vacancy in a two-dimensional crystal. Technical Physics Letters, 2014, 40, 657-661.	0.7	19
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	Family of Two-Dimensional Transition Metal Dichlorides: Fundamental Properties, Structural Defects, and Environmental Stability. Journal of Physical Chemistry Letters, 2022, 13, 2165-2172.	4.6	19
22	Exploring Mechanisms of Hydration and Carbonation of MgO and Mg(OH) ₂ in Reactive Magnesium Oxide-Based Cements. Journal of Physical Chemistry C, 2022, 126, 6196-6206.	3.1	18
23	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
24	Energy exchange between discrete breathers in crystal with NaCl structure. Technical Physics Letters, 2013, 39, 618-620.	0.7	15
25	Properties of moving discrete breathers in a monoatomic two-dimensional crystal. Journal of Experimental and Theoretical Physics, 2014, 119, 766-771.	0.9	13
26	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
27	Firstâ€Principles Study of Interaction of Bismuthene with Small Gas Molecules. ChemistrySelect, 2019, 4, 10928-10933.	1.5	12
28	In-situ quantification and density functional theory elucidation of phase transformation in carbon steel during quenching and partitioning. Acta Materialia, 2021, 221, 117361.	7.9	12
29	Synthesis and Characterization of the Ternary Nitride Semiconductor Zn ₂ VN ₃ : Theoretical Prediction, Combinatorial Screening, and Epitaxial Stabilization. Chemistry of Materials, 2021, 33, 9306-9316.	6.7	12
30	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
31	Nickel nanoparticle-activated MoS ₂ for efficient visible light photocatalytic hydrogen evolution. Nanoscale, 2022, 14, 8601-8610.	5.6	11
32	Discrete breathers in crystals with the NaCl structure. Russian Physics Journal, 2013, 56, 180-191.	0.4	10
33	The first-principles study of the adsorption of NH3, NO, and NO2 gas molecules on InSe-like phosphorus carbide. New Journal of Chemistry, 2020, 44, 9377-9381.	2.8	9
34	Impact of various dopant elements on the electronic structure of Cu ₂ ZnSnS ₄ (CZTS) thin films: a DFT study. CrystEngComm, 2020, 22, 5786-5791.	2.6	8
35	Vacancy-Induced Niobate Perovskite-Tungsten Bronze Composite for Synergetic Tuning of Ferroelectricity and Band Gaps. Journal of Physical Chemistry C, 2021, 125, 8890-8898.	3.1	8
36	Unveiling interactions of non-metallic inclusions within advanced ultra-high-strength steel: A spectro-microscopic determination and first-principles elucidation. Scripta Materialia, 2021, 197, 113791.	5.2	8

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37	The interaction of two-dimensional α- and β-phosphorus carbide with environmental molecules: a DFT study. Physical Chemistry Chemical Physics, 2020, 22, 11307-11313.	2.8	6
38	Properties of discrete breathers in 2D and 3D Morse crystals. Letters on Materials, 2014, 4, 315-318.	0.7	6
39	Incorporation of Si atoms into CrCoNiFe high-entropy alloy: a DFT study. Journal of Physics Condensed Matter, 2021, 33, 135703.	1.8	5
40	The reason for existence of discrete breathers in 2D and 3D Morse crystals. Letters on Materials, 2016, 6, 221-226.	0.7	5
41	Numerical modeling of 3D discrete breathers in fcc Ni. Letters on Materials, 2016, 6, 304-308.	0.7	4
42	Adsorption of Common Transition Metal Atoms on Arsenene: A First-Principles Study. Russian Journal of Physical Chemistry A, 2019, 93, 1088-1092.	0.6	3
43	Discerning phase-matrices for individual nitride inclusions within ultra-high-strength steel: experiment driven DFT investigation. Physical Chemistry Chemical Physics, 2022, 24, 1456-1461.	2.8	3
44	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
45	Temperature dependence of high-energy atoms density in the crystal with NaCl structure. Letters on Materials, 2012, 2, 143-146.	0.7	2
46	Bending instability of few-layer graphene embedded in strained polymer matrix. Letters on Materials, 2018, 8, 278-281.	0.7	2
47	The equilibrium states of A 1â^'x B 1+x binary alloys in the hard-sphere and pair-binding model. Russian Physics Journal, 2012, 54, 1128-1136.	0.4	1
48	Strain and defects engineering of phosphorene. , 2017, , .		1
49	Simulation of energy transport in crystal with NaCl structure assisted by discrete breathers. Letters on Materials, 2017, 7, 77-80.	0.7	1
50	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
51	Theoretical aspects of sulfide and selenides: Structure, point defects, and electronic structure modifications. , 2022, , 57-79.		0