Udo SchwingenschlÃ¶gl

List of Publications by Year
in descending order

239 papers	11,822 citations	39113 52 h-index	35168 102 g-index
240 all docs	240 docs citations	240 times ranked	17088 citing authors

#	Article	IF	Citations
1	Interfaces between Pb-Free Double Perovskite Cs2NaBiI6 and MXenes Sc2CO2 and Sc2C(OH)2. Journal of Physical Chemistry Letters, 2022, 13, 851-856.	2.1	0
2	Wafer-scale single-crystal monolayer graphene grown on sapphire substrate. Nature Materials, 2022, 21, 740-747.	13.3	92
3	Mechanical Reliability of Fullerene/Tin Oxide Interfaces in Monolithic Perovskite/Silicon Tandem Cells. ACS Energy Letters, 2022, 7, 827-833.	8.8	25
4	An Ultrahighâ€Flux Nanoporous Graphene Membrane for Sustainable Seawater Desalination using Lowâ€Grade Heat. Advanced Materials, 2022, 34, e2109718.	11.1	25
5	Low-energy Ga₂O₃ polymorphs with low electron effective masses. Physical Chemistry Chemical Physics, 2022, 24, 7045-7049.	1.3	8
6	Chemical vapor deposition-grown nitrogen-doped grapheneâ€™s synthesis, characterization and applications. Npj 2D Materials and Applications, 2022, 6, .	3.9	29
7	Conversion of twisted light to twisted excitons using carbon nanotubes. Npj Computational Materials, 2022, 8, .	3.5	1
8	Production of Largeâ€Area Nucleusâ€Free Singleâ€Crystal Grapheneâ€Mesh Metamaterials with Zigzag Edges. Advanced Materials, 2022, 34, e2201253.	11.1	5
9	Monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mrow><mml:mi mathvariant="normal">C</mml:mi></mml:mrow></mml:mrow><mml:mn>5</mml:mn></mml:msub><mml:mrow><mml:mrow><mml:m mathvariant="normal">N</mml:mi></mml:mrow></mml:mrow></mml:math> : A Promising Building Block for the Anode of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mrow><mml:mrow><mml:mi mathvariant="normal">K</mml:	1.5	5
10	Unusual Activity of Rationally Designed Cobalt Phosphide/Oxide Heterostructure Composite for Hydrogen Production in Alkaline Medium. ACS Nano, 2022, 16, 3906-3916.	7.3	50
11	Reply to â€œComment on â€˜Origin of symmetry-forbidden high-order harmonic generation in the time-dependent Kohn-Sham formulationâ€™â€. Physical Review A, 2022, 105, .	1.0	0
12	Monolayer, Bilayer, and Bulk BSi as Potential Anode Materials of Liâ€Ion Batteries. ChemPhysChem, 2022, 23, .	1.0	4
13	Damp heatâ€“stable perovskite solar cells with tailored-dimensionality 2D/3D heterojunctions. Science, 2022, 376, 73-77.	6.0	366
14	Transport and confinement in bilayer chiral borophene. 2D Materials, 2022, 9, 025031.	2.0	5
15	Comment on â€œElectrical Switch of Poissonâ€™s Ratio in IVâ€“VI Monolayers via Pseudophase Transitionsâ€. Journal of Physical Chemistry Letters, 2022, 13, 3609-3610.	2.1	1
16	Excellent Thermoelectric Performance of the Metal Sulfide CuTaS₃. ACS Applied Energy Materials, 2022, 5, 7364-7370.	2.5	5
17	Efficient and stable perovskite-silicon tandem solar cells through contact displacement by MgF <i> _x </i>. Science, 2022, 377, 302-306.	6.0	141
18	The metallic C6S monolayer with high specific capacity for K-ion batteries. Materials Today Chemistry, 2022, 25, 100951.	1.7	3

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19	Tuneable Poissonâ€™s ratio of monolayer GeS and Ge2SSe. Extreme Mechanics Letters, 2022, , 101838.	2.0	0
20	A Cyclized Polyacrylonitrile Anode for Alkali Metal Ion Batteries. Angewandte Chemie - International Edition, 2021, 60, 1355-1363.	7.2	41
21	A Cyclized Polyacrylonitrile Anode for Alkali Metal Ion Batteries. Angewandte Chemie, 2021, 133, 1375-1383.	1.6	8
22	Bridging the interfacial gap in mixed-matrix membranes by nature-inspired design: precise molecular sieving with polymer-grafted metalâ€“organic frameworks. Journal of Materials Chemistry A, 2021, 9, 23793-23801.	5.2	41
23	Defining sulfonation limits of poly(ether-ether-ketone) for energy-efficient dehumidification. Journal of Materials Chemistry A, 2021, 9, 17740-17748.	5.2	7
24	Unique Omnidirectional Negative Poissonâ€™s Ratio in Î´-Phase Carbon Monochalcogenides. Journal of Physical Chemistry C, 2021, 125, 4133-4138.	1.5	39
25	Confined variational calculation of positronium-hydrogen scattering below the positronium excitation threshold. Physical Review A, 2021, 103, .	1.0	9
26	Multivalley Band Structure and Phonon-Glass Behavior of TlAgTe. ACS Applied Energy Materials, 2021, 4, 2174-2180.	2.5	5
27	Anisotropic Janus SiP₂ Monolayer as a Photocatalyst for Water Splitting. Journal of Physical Chemistry Letters, 2021, 12, 2464-2470.	2.1	49
28	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mi>M</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi>X</mml:mi></mml:math> Monolayers as Anode Materials for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Li</mml:mi></mml:math> Ion Batteries. Physical Review Applied, 2021, 15, .	1.5	13
29	Effective Doping of Square/Octagonâ€Phase Arsenene by Adsorption of Organic Molecules. Advanced Theory and Simulations, 2021, 4, 2000300.	1.3	1
30	Structure Prototype Outperforming MXenes in Stability and Performance in Metalâ€Ion Batteries: A High Throughput Study. Advanced Energy Materials, 2021, 11, 2003633.	10.2	111
31	Two-Dimensional Tetrahex-GeC₂: A Material with Tunable Electronic and Optical Properties Combined with Ultrahigh Carrier Mobility. ACS Applied Materials & Interfaces, 2021, 13, 14489-14496.	4.0	15
32	Borophene-Based Three-Dimensional Porous Structures as Anode Materials for Alkali Metal-Ion Batteries with Ultrahigh Capacity. Chemistry of Materials, 2021, 33, 2976-2983.	3.2	20
33	Origin of symmetry-forbidden high-order harmonic generation in the time-dependent Kohn-Sham formulation. Physical Review A, 2021, 103, .	1.0	2
34	Pd₄S₃Se₃, Pd₄S₃Te₃, and Pd₄Se₃Te₃: Candidate Two-Dimensional Janus Materials for Photocatalytic Water Splitting. Chemistry of Materials, 2021, 33, 4128-4134.	3.2	59
35	First principles calculations of the structural, electronic, magnetic, and thermodynamic properties of the Nd2MgGe2 and Gd2MgGe2 intermetallic compounds. Scientific Reports, 2021, 11, 10870.	1.6	5
36	Concurrent cationic and anionic perovskite defect passivation enables 27.4% perovskite/silicon tandems with suppression of halide segregation. Joule, 2021, 5, 1566-1586.	11.7	119

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37	Sustained Solar-Powered Electrocatalytic H₂ Production by Seawater Splitting Using Two-Dimensional Vanadium Disulfide. ACS Sustainable Chemistry and Engineering, 2021, 9, 8572-8580.	3.2	10
38	Two Phases of Monolayer Tantalum Sulfide on Au(111). ACS Nano, 2021, 15, 13516-13525.	7.3	10
39	Chiral Helimagnetism and Oneâ€Dimensional Magnetic Solitons in a Crâ€Intercalated Transition Metal Dichalcogenide. Advanced Materials, 2021, 33, e2101131.	11.1	40
40	Large Magnetocrystalline Anisotropy and Giant Coercivity in the Ferrimagnetic Double Perovskite Lu₂NiIrO₆. Nano Letters, 2021, 21, 6807-6812.	4.5	13
41	Ultrahigh Carrier Mobility in the Two-Dimensional Semiconductors B₈Si₄, B₈Ge₄, and B₈Sn₄. Chemistry of Materials, 2021, 33, 6475-6483.	3.2	104
42	Semimetallic 2D Alkynyl Carbon Materials with Distorted Type I Dirac Cones. Journal of Physical Chemistry C, 2021, 125, 18022-18030.	1.5	7
43	Lattice-matched III-nitride structures comprising BAlN, BGaN, and AlGaN for ultraviolet applications. Materials Research Express, 2021, 8, 086202.	0.8	6
44	Designing graphene origami structures with a giant isotropic negative coefficient of thermal expansion. Extreme Mechanics Letters, 2021, 47, 101357.	2.0	3
45	Dipole-induced Ohmic contacts between monolayer Janus MoSSe and bulk metals. Npj 2D Materials and Applications, 2021, 5, .	3.9	18
46	Modeling of n â€Alkanes on Calcite/Dolomite by Molecular Dynamics Simulations and Firstâ€Principles Calculations. Advanced Theory and Simulations, 2021, 4, 2100226.	1.3	4
47	Janus monolayers of magnetic transition metal dichalcogenides as an all-in-one platform for spin-orbit torque. Physical Review B, 2021, 104, .	1.1	13
48	Accordionâ€Like Carbon with High Nitrogen Doping for Fast and Stable K Ion Storage. Advanced Energy Materials, 2021, 11, 2101928.	10.2	88
49	Control of spinâ€“charge conversion in van der Waals heterostructures. APL Materials, 2021, 9, .	2.2	20
50	Molecular Dynamics Modeling of Kaolinite Particle Associations. Journal of Physical Chemistry C, 2021, 125, 24126-24136.	1.5	7
51	Inducing Half-Metallicity in Monolayer MoSi₂N₄. ACS Omega, 2021, 6, 30371-30375.	1.6	17
52	Structure of monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>2</mml:mn><mml:mi>H</mml:mi></mml:mrow><mml:n mathvariant="normal">TaS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> on Au(111). Physical Review B, 2021, 104, .	1.1	6
53	BC₆P Monolayer: Isostructural and Isoelectronic Analogues of Graphene with Desirable Properties for K-Ion Batteries. Chemistry of Materials, 2021, 33, 9262-9269.	3.2	11
54	Molecular doping of blue phosphorene: a first-principles investigation. Journal of Physics Condensed Matter, 2020, 32, 055501.	0.7	14

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55	Beryllene: A Promising Anode Material for Na- and K-Ion Batteries with Ultrafast Charge/Discharge and High Specific Capacity. Journal of Physical Chemistry Letters, 2020, 11, 9051-9056.	2.1	78
56	Monolayer Ag₂S: Ultralow Lattice Thermal Conductivity and Excellent Thermoelectric Performance. ACS Applied Energy Materials, 2020, 3, 10147-10153.	2.5	14
57	Molecular engineering of high-performance nanofiltration membranes from intrinsically microporous poly(ether-ether-ketone). Journal of Materials Chemistry A, 2020, 8, 24445-24454.	5.2	34
58	MXene-Modulated Electrode/SnO₂ Interface Boosting Charge Transport in Perovskite Solar Cells. ACS Applied Materials & Interfaces, 2020, 12, 53973-53983.	4.0	71
59	Quantum dots in AA-stacked bilayer graphene. Physical Review B, 2020, 102, .	1.1	4
60	Selective Toluene Detection with Mo₂CT_{<i>x</i>} MXene at Room Temperature. ACS Applied Materials & Interfaces, 2020, 12, 57218-57227.	4.0	83
61	Graphene origami structures with superflexibility and highly tunable auxeticity. Physical Review B, 2020, 102, .	1.1	26
62	Chemical Separation: Finely Tuned Submicroporous Thinâ€Film Molecular Sieve Membranes for Highly Efficient Fluid Separations (Adv. Mater. 22/2020). Advanced Materials, 2020, 32, 2070171.	11.1	2
63	Tunable magnetic anisotropy in Crâ€"trihalide Janus monolayers. Journal of Physics Condensed Matter, 2020, 32, 355702.	0.7	21
64	Direct Pyrolysis of Supermolecules: An Ultrahigh Edgeâ€Nitrogen Doping Strategy of Carbon Anodes for Potassiumâ€Ion Batteries. Advanced Materials, 2020, 32, e2000732.	11.1	164
65	B₂P₆: A Two-Dimensional Anisotropic Janus Material with Potential in Photocatalytic Water Splitting and Metal-Ion Batteries. Chemistry of Materials, 2020, 32, 4795-4800.	3.2	142
66	Transition from Schottky to Ohmic contacts in Janus MoSSe/germanene heterostructures. Nanoscale, 2020, 12, 11448-11454.	2.8	37
67	Selective Electrocatalytic Oxidation of Biomassâ€Derived 5â€Hydroxymethylfurfural to 2,5â€Diformylfuran: from Mechanistic Investigations to Catalyst Recovery. ChemSusChem, 2020, 13, 3060-3060.	3.6	3
68	Graphene Origami with Highly Tunable Coefficient of Thermal Expansion. ACS Nano, 2020, 14, 8969-8974.	7.3	36
69	Gas Sensing Performance of Pristine and Monovacant C6BN Monolayers Evaluated by Density Functional Theory and the Nonequilibrium Greenâ€™s Function Formalism. Journal of Physical Chemistry C, 2020, 124, 5853-5860.	1.5	18
70	Effects of gas adsorption on monolayer Si₂BN and implications for sensing applications. Journal of Physics Condensed Matter, 2020, 32, 355602.	0.7	8
71	Flexible C₆BN Monolayers As Promising Anode Materials for High-Performance K-Ion Batteries. ACS Applied Materials & Interfaces, 2020, 12, 30731-30739.	4.0	69
72	Mechanism of wettability alteration of the calcite {101Ì„4} surface. Physical Chemistry Chemical Physics, 2020, 22, 15365-15372.	1.3	17

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73	Identification and Resolution of Unphysical Multielectron Excitations in the Real-Time Time-Dependent Kohn-Sham Formulation. Physical Review Letters, 2020, 124, 026402.	2.9	4
74	Complex three-dimensional graphene structures driven by surface functionalization. Nanoscale, 2020, 12, 10172-10179.	2.8	18
75	Selective Electrocatalytic Oxidation of Biomassâ€Derived 5â€Hydroxymethylfurfural to 2,5â€Diformylfuran: from Mechanistic Investigations to Catalyst Recovery. ChemSusChem, 2020, 13, 3127-3136.	3.6	45
76	Finely Tuned Submicroporous Thinâ€Film Molecular Sieve Membranes for Highly Efficient Fluid Separations. Advanced Materials, 2020, 32, e2001132.	11.1	59
77	Confined variational calculation of o -Psâ€"He scattering properties. Physical Review A, 2020, 101, .	1.0	11
78	Sensitivity enhancement of stanene towards toxic SO2 and H2S. Applied Surface Science, 2019, 495, 143622.	3.1	17
79	Scalable Synthesis of Amphiphilic Copolymers for CO₂- and Water-Selective Membranes: Effect of Copolymer Composition and Chain Length. Macromolecules, 2019, 52, 6213-6226.	2.2	28
80	First-principles methodology for determining the angular momentum of excitons. Physical Review B, 2019, 100, .	1.1	1
81	Suppressing Xâ€Migrations and Enhancing the Phase Stability of Cubic FAPbX₃ (X = Br, I). Advanced Energy Materials, 2019, 9, 1901411.	10.2	20
82	Copper Thiocyanate and Copper Selenocyanate Hole Transport Layers: Determination of Band Offsets with Silicon and Hybrid Perovskites from First Principles. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1900328.	1.2	25
83	Electronic States at the Zigzag Edges of Graphene Terraces. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1900513.	1.2	0
84	Diffusion equations expressed in molar fractions: Theory and application to ionic diffusion and demixing. Physical Review E, 2019, 100, 042124.	0.8	1
85	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>S</mml:mi></mml:math> -wave elastic scattering of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>o</mml:mi></mml:math> -Ps from <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> at low energy. Physical Review A, 2019, 100, .	1.0	14
86	Point Defects in Blue Phosphorene. Chemistry of Materials, 2019, 31, 8129-8135.	3.2	86
87	Density Functional Theory Analysis of Gas Adsorption on Monolayer and Few Layer Transition Metal Dichalcogenides: Implications for Sensing. ACS Applied Nano Materials, 2019, 2, 6076-6080.	2.4	49
88	Pressure-induced conduction band convergence in the thermoelectric ternary chalcogenide CuBiS₂. Physical Chemistry Chemical Physics, 2019, 21, 662-673.	1.3	15
89	New Paradigm for Gas Sensing by Two-Dimensional Materials. Journal of Physical Chemistry C, 2019, 123, 13104-13109.	1.5	24
90	Abâ€Initio Investigation of the Band Alignment Between Cu 2 ZnSnS 4 and Different Buffer Materials (Al) Tj ETQq0 0 0 rgBT /Overlock 1	1.2	3

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91	Ultralow Lattice Thermal Conductivity and Thermoelectric Properties of Monolayer Tl₂O. ACS Applied Energy Materials, 2019, 2, 3004-3008.	2.5	52
92	Highâ€Performance Fieldâ€Effect Transistors Based on Î±P and Î²P. Advanced Materials, 2019, 31, 1807810.	11.1	9
93	Zrâ€Doped Indium Oxide (IZRO) Transparent Electrodes for Perovskiteâ€Based Tandem Solar Cells. Advanced Functional Materials, 2019, 29, 1901741.	7.8	124
94	Metal-induced gap states in passivating metal/silicon contacts. Applied Physics Letters, 2019, 114, .	1.5	25
95	A 0D Leadâ€Free Hybrid Crystal with Ultralow Thermal Conductivity. Advanced Functional Materials, 2019, 29, 1809166.	7.8	32
96	Recent Insights from Computational Materials Chemistry into Interfaces Relevant to Enhanced Oil Recovery. Advanced Theory and Simulations, 2019, 2, 1800183.	1.3	4
97	Origin of the transition entropy in vanadium dioxide. Physical Review B, 2019, 99, .	1.1	20
98	Computational Tuning of the Paddlewheel tcb-MOF Family for Advanced Methane Sorption. ACS Applied Energy Materials, 2019, 2, 222-231.	2.5	4
99	Highways for water molecules: Interplay between nanostructure and water vapor transport in block copolymer membranes. Journal of Membrane Science, 2019, 572, 641-649.	4.1	51
100	Highly Sensitive Sensing of NO and NO₂ Gases by Monolayer C₃N. Advanced Theory and Simulations, 2018, 1, 1700008.	1.3	43
101	Two-Dimensional Tellurene as Excellent Thermoelectric Material. ACS Applied Energy Materials, 2018, 1, 1950-1954.	2.5	93
102	Metallicity at interphase boundaries due to polar catastrophe induced by charge density discontinuity. NPG Asia Materials, 2018, 10, e469-e469.	3.8	3
103	Silicene on Monolayer PtSe₂: From Strong to Weak Binding via NH₃ Intercalation. ACS Applied Materials & Interfaces, 2018, 10, 4266-4270.	4.0	10
104	Alloying as a Route to Monolayer Transition Metal Dichalcogenides with Improved Optoelectronic Performance: Mo(S_{1â€“<i>x</i>}Se_{<i>x</i>})₂ and Mo_{1â€“<i>y</i>}W_{<i>y</i>}S₂. ACS Applied Energy Materials, 2018, 1, 2208-2214.	2.5	17
105	Theoretical study on cation codoped SrTiO₃ photocatalysts for water splitting. Journal of Materials Chemistry A, 2018, 6, 24342-24349.	5.2	20
106	Band Gap Control in Bilayer Graphene by Co-Doping with B-N Pairs. Scientific Reports, 2018, 8, 17689.	1.6	24
107	Room-Temperature-Sputtered Nanocrystalline Nickel Oxide as Hole Transport Layer for pâ€“iâ€“n Perovskite Solar Cells. ACS Applied Energy Materials, 2018, 1, 6227-6233.	2.5	88
108	MXene/Graphene Heterostructures as High-Performance Electrodes for Li-Ion Batteries. ACS Applied Materials & Interfaces, 2018, 10, 32867-32873.	4.0	149

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109	Molecular dynamics of Middle East Respiratory Syndrome Coronavirus (MERS CoV) fusion heptad repeat trimers. Computational Biology and Chemistry, 2018, 75, 205-212.	1.1	15
110	Potential of B/Alâ€Doped Silicene Electrodes in Na/Kâ€Ion Batteries. Advanced Theory and Simulations, 2018, 1, 1800017.	1.3	12
111	Valley-dependent current generation in nanotubes by twisted light. Physical Review B, 2018, 98, .	1.1	2
112	Effects of oxygen vacancies on the electronic structure of the (LaVO₃)₆/SrVO₃ superlattice: a computational study. New Journal of Physics, 2018, 20, 073011.	1.2	5
113	Electronic Reconstruction in (LaVO₃)<i>_m</i>/SrVO₃ (<i>_m</i> = 5, 6) Superlattices. Advanced Materials Interfaces, 2018, 5, 1701169.	1.9	7
114	Stacking Effects in van der Waals Heterostructures of Silicene and Hexagonal Boron Nitride. Advanced Theory and Simulations, 2018, 1, 1800083.	1.3	12
115	Topological characterization of carbon nanotubes. Journal of Physics Condensed Matter, 2018, 30, 335301.	0.7	1
116	Thermoelectric Materials Under Pressure. Physica Status Solidi - Rapid Research Letters, 2018, 12, 1800083.	1.2	13
117	Adsorption of the Gas Molecules NH₃, NO, NO₂, and CO on Borophene. Journal of Physical Chemistry C, 2018, 122, 14665-14670.	1.5	91
118	Temperature-dependent magnetic anisotropy in the layered magnetic semiconductors <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Cr</mml:mi><mml:msub><mml:mi mathvariant="normal">I</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>CrB</mml:mi><mml:msub><mml:mi mathvariant="normal">r</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physi	0.9	70
119	Two-Dimensional SnO Anodes with a Tunable Number of Atomic Layers for Sodium Ion Batteries. Nano Letters, 2017, 17, 1302-1311.	4.5	118
120	Interaction of Monovacancies in Graphene. Journal of Physical Chemistry C, 2017, 121, 2459-2465.	1.5	1
121	Transport properties of hydrogen passivated silicon nanotubes and silicon nanotube field effect transistors. Journal of Materials Chemistry C, 2017, 5, 1409-1413.	2.7	7
122	Active Edge Sites Engineering in Nickel Cobalt Selenide Solid Solutions for Highly Efficient Hydrogen Evolution. Advanced Energy Materials, 2017, 7, 1602089.	10.2	171
123	Intrinsic Defects and H Doping in WO3. Scientific Reports, 2017, 7, 40882.	1.6	65
124	Amorphous NiFe-OH/NiFeP Electrocatalyst Fabricated at Low Temperature for Water Oxidation Applications. ACS Energy Letters, 2017, 2, 1035-1042.	8.8	505
125	Lead monoxide: a two-dimensional ferromagnetic semiconductor induced by hole-doping. Journal of Materials Chemistry C, 2017, 5, 4520-4525.	2.7	17
126	O vacancy formation in (Pr/Gd)BaCo₂O_{5.5} and the role of antisite defects. Physical Chemistry Chemical Physics, 2017, 19, 11455-11459.	1.3	3

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127	Electrocatalysts: In Operando Self-Healing of Perovskite Electrocatalysts: A Case Study of SrCoO3 for the Oxygen Evolution Reaction (Part. Part. Syst. Charact. 4/2017). Particle and Particle Systems Characterization, 2017, 34, .	1.2	1
128	Electronic Properties of Grapheneâ€“PtSe₂ Contacts. ACS Applied Materials & Interfaces, 2017, 9, 15809-15813.	4.0	41
129	Superior selectivity and sensitivity of blue phosphorus nanotubes in gas sensing applications. Journal of Materials Chemistry C, 2017, 5, 5365-5371.	2.7	23
130	Thermoelectric properties of the misfit cobaltate Ca3Co4O9. Applied Physics Letters, 2017, 110, .	1.5	9
131	In Operando Selfâ€Healing of Perovskite Electrocatalysts: A Case Study of SrCoO₃ for the Oxygen Evolution Reaction. Particle and Particle Systems Characterization, 2017, 34, 1600280.	1.2	10
132	O deficient LaAlO3/SrTiO3(110) and (001) superlattices under hydrostatic pressure: a comparative first principles study. Journal of Materials Chemistry C, 2017, 5, 3336-3342.	2.7	0
133	Hexagonal graphene quantum dots. Physica Status Solidi - Rapid Research Letters, 2017, 11, 1600226.	1.2	5
134	Superior Gas Sensing Properties of Monolayer PtSe₂. Advanced Materials Interfaces, 2017, 4, 1600911.	1.9	110
135	Potential of transition metal atoms embedded in buckled monolayer g-C₃N₄ as single-atom catalysts. Physical Chemistry Chemical Physics, 2017, 19, 30069-30077.	1.3	78
136	First-principles prediction of Tl/SiC for valleytronics. Journal of Materials Chemistry C, 2017, 5, 10427-10433.	2.7	12
137	Spin-Charge Separation in Finite Length Metallic Carbon Nanotubes. Nano Letters, 2017, 17, 6747-6751.	4.5	1
138	Polybenzimidazole-based mixed membranes with exceptionally high water vapor permeability and selectivity. Journal of Materials Chemistry A, 2017, 5, 21807-21819.	5.2	33
139	Ultralow lattice thermal conductivity in monolayer C₃N as compared to graphene. Journal of Materials Chemistry A, 2017, 5, 20407-20411.	5.2	60
140	Thermoelectric Properties of the XCoSb (X: Ti,Zr,Hf) Halfâ€Heusler alloys. Physica Status Solidi (B): Basic Research, 2017, 254, 1700419.	0.7	14
141	Quantum Transport Through Tunable Molecular Diodes. Scientific Reports, 2017, 7, 7324.	1.6	6
142	Functionalized NbS2 as cathode for Li- and Na-ion batteries. Applied Physics Letters, 2017, 111, .	1.5	19
143	Spin-polarized ballistic conduction through correlated Au-NiMnSb-Au heterostructures. Physical Review B, 2017, 96, .	1.1	6
144	Arsenene and Antimonene: Two-Dimensional Materials with High Thermoelectric Figures of Merit. Physical Review Applied, 2017, 8, .	1.5	120

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145	A Route to Permanent Valley Polarization in Monolayer MoS₂. Advanced Materials, 2017, 29, 1600970.	11.1	109
146	Elemental Two-Dimensional Materials Beyond Graphene. ChemistrySelect, 2017, 2, .	0.7	0
147	Tailoring the Electronic and Magnetic Properties of Two-Dimensional Silicon Carbide Sheets and Ribbons by Fluorination. Journal of Physical Chemistry C, 2016, 120, 15407-15414.	1.5	8
148	Manganite/Cuprate Superlattice as Artificial Reentrant Spin Glass. Advanced Materials Interfaces, 2016, 3, 1500676.	1.9	22
149	Spinâ€polarized electron gas in Co₂<i>M</i> Si/SrTiO₃ (<i>M</i> = Ti, V, Cr, Mn,) Tj ETQq1 1 0.784314 rgBT /	1.2	1
150	Optical properties of Al nanostructures from time dependent density functional theory. Journal of Chemical Physics, 2016, 144, 134305.	1.2	6
151	Silicene: Recent theoretical advances. Applied Physics Reviews, 2016, 3, .	5.5	94
152	Quasi-freestanding graphene on Ni(111) by Cs intercalation. Scientific Reports, 2016, 6, 26753.	1.6	14
153	Curvature effects in two-dimensional optical devices inspired by transformation optics. Applied Physics Letters, 2016, 109, 201105.	1.5	1
154	Electron dominated thermoelectric response in MNiSn (M: Ti, Zr, Hf) half-Heusler alloys. Physical Chemistry Chemical Physics, 2016, 18, 14017-14022.	1.3	25
155	S-functionalized MXenes as electrode materials for Li-ion batteries. Applied Materials Today, 2016, 5, 19-24.	2.3	89
156	Role of interlayer coupling for the power factor ofCuSbS2andCuSbSe2. Physical Review B, 2016, 94, .	1.1	12
157	Vacancy formation in MoO₃: hybrid density functional theory and photoemission experiments. Journal of Materials Chemistry C, 2016, 4, 9526-9531.	2.7	24
158	Thermoelectric Response in Single Quintuple Layer Bi₂Te₃. ACS Energy Letters, 2016, 1, 875-879.	8.8	52
159	Nanotubes based on monolayer blue phosphorus. Physical Review B, 2016, 94, .	1.1	28
160	Extended Moment Formation in Monolayer WS₂ Doped with 3d Transition-Metals. ACS Applied Materials & Interfaces, 2016, 8, 23886-23890.	4.0	23
161	SnSe₂ 2D Anodes for Advanced Sodium Ion Batteries. Advanced Energy Materials, 2016, 6, 1601188.	10.2	243
162	Silicene for Na-ion battery applications. 2D Materials, 2016, 3, 035012.	2.0	82

#	Article	IF	Citations
163	Polar catastrophe at the MgO(100)/SnO₂(110) interface. Journal of Materials Chemistry C, 2016, 4, 11129-11134.	2.7	3
164	Magnetism in 3d transition metal doped SnO. Journal of Materials Chemistry C, 2016, 4, 8947-8952.	2.7	25
165	Tunable optical absorption in silicene molecules. Journal of Materials Chemistry C, 2016, 4, 7387-7390.	2.7	10
166	Formation and Migration of Oxygen Vacancies in SrCoO₃ and Their Effect on Oxygen Evolution Reactions. ACS Catalysis, 2016, 6, 5565-5570.	5.5	96
167	Electronic phase transitions under hydrostatic pressure in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaMnO</mml:mi><mml:mn>3</mml:mn></mml:msub></ bilayers sandwiched between<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaAlO</mml:mi><mml:mn>3</mml:mn></mml:msub><m Physical Review B, 2016, 93, .	1.1	5
168	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>k</mml:mi></mml:math>-asymmetric spin splitting at the interface between transition metal ferromagnets and heavy metals. Physical Review B, 2016, 93, .	1.1	48
169	Plasma-Assisted Synthesis of NiCoP for Efficient Overall Water Splitting. Nano Letters, 2016, 16, 7718-7725.	4.5	1,079
170	Floquet edge states in germanene nanoribbons. Scientific Reports, 2016, 6, 31821.	1.6	16
171	Transmission comb of a distributed Bragg reflector with two surface dielectric gratings. Scientific Reports, 2016, 6, 21125.	1.6	4
172	Dynamics of single photon transport in a one-dimensional waveguide two-point coupled with a Jaynes-Cummings system. Scientific Reports, 2016, 6, 33867.	1.6	26
173	Defect engineering of the electronic transport through cuprous oxide interlayers. Scientific Reports, 2016, 6, 27049.	1.6	7
174	CO₂ capture by Liâ€functionalized silicene. Physica Status Solidi - Rapid Research Letters, 2016, 10, 458-461.	1.2	3
175	Formation of Metallic States between Insulating SnO and SnO₂. Advanced Materials Interfaces, 2016, 3, 1500334.	1.9	2
176	Ultrafast and Highly Reversible Sodium Storage in Zincâ€Antimony Intermetallic Nanomaterials. Advanced Functional Materials, 2016, 26, 543-552.	7.8	81
177	Intrinsic defect processes and O migration in PrBa(Co/Fe)₂O_{5.5}. Journal of Materials Chemistry A, 2016, 4, 3560-3564.	5.2	6
178	Thermoelectric Performance of the MXenes M₂CO₂ (M = Ti, Zr, or Hf). Chemistry of Materials, 2016, 28, 1647-1652.	3.2	132
179	Thermal conductivity of bulk and monolayer MoS ₂. Europhysics Letters, 2016, 113, 36002.	0.7	117
180	Silicene/germanene on MgX₂(X = Cl, Br, and I) for Li-ion battery applications. Nanoscale, 2016, 8, 7272-7277.	2.8	61

#	Article	IF	Citations
181	Two-Dimensional MnO2/Graphene Interface: Half-Metallicity and Quantum Anomalous Hall State. Journal of Physical Chemistry C, 2016, 120, 2119-2125.	1.5	29
182	Heterostructures of transition metal dichalcogenides. Physical Review B, 2015, 92, .	1.1	190
183	Transparent SnOâ€“SnO₂ pâ€“n Junction Diodes for Electronic and Sensing Applications. Advanced Materials Interfaces, 2015, 2, 1500374.	1.9	31
184	Silicene on MoS ₂ : role of the van der Waals interaction. 2D Materials, 2015, 2, 045004.	2.0	22
185	Ultrafast palladium diffusion in germanium. Journal of Materials Chemistry A, 2015, 3, 3832-3838.	5.2	14
186	Thermoelectric Response of Bulk and Monolayer MoSe₂ and WSe₂. Chemistry of Materials, 2015, 27, 1278-1284.	3.2	308
187	Absorption Spectra of CuGaSe₂ and CuInSe₂ Semiconducting Nanoclusters. Journal of Physical Chemistry C, 2015, 119, 22732-22736.	1.5	4
188	A global view of the phase transitions of SnO₂ in rechargeable batteries based on results of high throughput calculations. Journal of Materials Chemistry A, 2015, 3, 19483-19489.	5.2	21
189	Is NiCo₂S₄ Really a Semiconductor?. Chemistry of Materials, 2015, 27, 6482-6485.	3.2	203
190	Pressure controlled transition into a self-induced topological superconducting surface state. Scientific Reports, 2015, 4, 4025.	1.6	9
191	Structural and magnetic properties of Gd-doped ZnO. Journal of Materials Chemistry C, 2014, 2, 10331-10336.	2.7	26
192	Effects of heavy metal adsorption on silicene. Physica Status Solidi - Rapid Research Letters, 2014, 8, 685-687.	1.2	31
193	Giant Rashba spin splitting in Bi₂ Se₃ :Tl. Physica Status Solidi - Rapid Research Letters, 2014, 8, 849-852.	1.2	3
194	Topological phases of silicene and germanene in an external magnetic field: Quantitative results. Physica Status Solidi - Rapid Research Letters, 2014, 8, 353-356.	1.2	8
195	Anisotropic O vacancy formation and diffusion in LaMnO₃. Journal of Materials Chemistry A, 2014, 2, 19733-19737.	5.2	16
196	Possible mechanism for d⁰ ferromagnetism mediated by intrinsic defects. RSC Advances, 2014, 4, 50759-50764.	1.7	43
197	Ferromagnetism in Cr-doped passivated AlN nanowires. Journal of Materials Chemistry A, 2014, 2, 9287-9290.	5.2	8
198	Strain engineering of WS₂, WSe₂, and WTe₂. RSC Advances, 2014, 4, 34561.	1.7	279

#	Article	IF	Citations
199	Thermoelectric performance enhancement of SrTiO3 by Pr doping. Journal of Materials Chemistry A, 2014, 2, 10379.	5.2	21
200	Tuning the optical response in carbon doped boron nitride nanodots. Journal of Materials Chemistry C, 2014, 2, 8322-8327.	2.7	14
201	LaBiTe3: An unusual thermoelectric material. Physica Status Solidi - Rapid Research Letters, 2014, 08, 805-808.	1.2	10
202	Valley polarization in magnetically doped single-layer transition-metal dichalcogenides. Physical Review B, 2014, 89, .	1.1	181
203	Superior thermoelectric response in the 3R phases of hydrated NaxRhO2. Scientific Reports, 2014, 4, 4390.	1.6	9
204	Major enhancement of the thermoelectric performance in Pr/Nb-doped SrTiO3 under strain. Applied Physics Letters, 2013, 103, .	1.5	25
205	Van der Waals epitaxial growth of MoS2 on SiO2/Si by chemical vapor deposition. RSC Advances, 2013, 3, 17287.	1.7	41
206	Catalytically favorable surface patterns in Ptâ€"Au nanoclusters. RSC Advances, 2013, 3, 15350.	1.7	8
207	Exotic High Activity Surface Patterns in PtAu Nanoclusters. Journal of Physical Chemistry C, 2013, 117, 9275-9280.	1.5	10
208	Half-metallic perovskite superlattices with colossal thermoelectric figure of merit. Journal of Materials Chemistry A, 2013, 1, 8406.	5.2	12
209	Oxygen adsorption and dissociation during the oxidation of monolayer Ti2C. Journal of Materials Chemistry A, 2013, 1, 13672.	5.2	77
210	Tuning the chemical activity through PtAu nanoalloying: a first principles study. Journal of Materials Chemistry A, 2013, 1, 9885.	5.2	19
211	Topological Phase Diagrams of Bulk and Monolayer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>TiS</mml:mi><mml:mrow><mml:mn>2</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml: Physical Review Letters, 2013, 110, 077202.	2.9	41
212	First-principles analysis of MoS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>/Ti<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>C and MoS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:	1.1	166
213	Surface antiferromagnetism and incipient metal-insulator transition in strained manganite films. Physical Review B, 2013, 87, .	1.1	11
214	Thermoelectric performance of electron and hole doped PtSb2. Journal of Applied Physics, 2013, 113, .	1.1	13
215	Virtual half-metallicity at the CoS2/FeS2 interface induced by strain. RSC Advances, 2013, 3, 4518.	1.7	9
216	Spin-orbitâ€"induced spin splittings in polar transition metal dichalcogenide monolayers. Europhysics Letters, 2013, 102, 57001.	0.7	334

#	Article	IF	Citations
217	Lattice relaxation and ferromagnetic character of (LaVO 3) m /SrVO 3 superlattices. Europhysics Letters, 2013, 103, 37003.	0.7	3
218	Molecular distortion and charge transfer effects in ZnPc/Cu(111). Scientific Reports, 2013, 3, .	1.6	19
219	Anomalous positive flatband voltage shifts in metal gate stacks containing rare-earth oxide capping layers. Applied Physics Letters, 2012, 100, 102111.	1.5	3
220	Role of the dimensionality of the [GaX]2 network in the Zintl phases EuGa2X2. Journal of Applied Physics, 2012, 112, 103714.	1.1	4
221	Enhanced carrier density in Nb-doped SrTiO3 thermoelectrics. Journal of Applied Physics, 2012, 111, .	1.1	33
222	Strain-activated edge reconstruction of graphene nanoribbons. Physical Review B, 2012, 85, .	1.1	25
223	Anomalous enhancement of the thermoelectric figure of merit by V co-doping of Nb-SrTiO3. Applied Physics Letters, 2012, 100, 193110.	1.5	9
224	Long-range interactions between excited helium and alkali-metal atoms. Physical Review A, 2012, 86, .	1.0	9
225	Mechanical failure of zigzag graphene nanoribbons under tensile strain induced by edge reconstruction. Journal of Materials Chemistry, 2012, 22, 24676.	6.7	11
226	A route to ultrathin quantum gases at polar perovskite heterointerfaces. Physica Status Solidi - Rapid Research Letters, 2012, 6, 373-375.	1.2	0
227	Optical and photocatalytic properties of two-dimensional MoS2. European Physical Journal B, 2012, 85, 1.	0.6	121
228	Experimental and theoretical investigation of the effect of SiO2 content in gate dielectrics on work function shift induced by nanoscale capping layers. Applied Physics Letters, 2012, 101, .	1.5	4
229	Spectral Analysis of Quantum-Dash Lasers: Effect of Inhomogeneous Broadening of the Active-Gain Region. IEEE Journal of Quantum Electronics, 2012, 48, 608-615.	1.0	10
230	Theoretical observation of two state lasing from InAs/InP quantum-dash lasers. , 2011, , .		0
231	Modeling the lasing spectra of InAs/InP Quantum dash lasers. Applied Physics Letters, 2011, 98, 101105.	1.5	14
232	Ab initio investigation on the magnetic ordering in Gd doped ZnO. Journal of Applied Physics, 2011, 109, 083929.	1.1	37
233	Giant spin-orbit-induced spin splitting in two-dimensional transition-metal dichalcogenide semiconductors. Physical Review B, 2011, 84, .	1.1	1,306
234	Structural Properties of Iron Nitride on Cu(100): an Ab-initio Molecular Dynamics study. Materials Research Society Symposia Proceedings, 2011, 1290, 1.	0.1	2

#	Article	IF	Citations
235	Electronic Structure and Optical Properties Of EuIn[sub 2]P[sub 2]. AIP Conference Proceedings, 2011, , .	0.3	1
236	A route to strong p-doping of epitaxial graphene on SiC. Applied Physics Letters, 2010, 97, 193304.	1.5	22
237	Effect of active medium inhomogeneity on lasing characteristics of InAs/InP quantum-dash lasers. , 2010, , .		1
238	The influence of quantum-dash height on the differential gain and linewidth enhancement factor of InAs/InP quantum-dash lasers. , 2010, , .		0
239	Prediction of femtosecond oscillations in the transient current of a quantum dot in the Kondo regime. Physical Review B, 2010, 82, .	1.1	10