Valentino R Cooper

List of Publications by Year
in descending order

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119 papers	9,946 citations	81900 39 h-index	34986 98 g-index
123 all docs	123 docs citations	123 times ranked	15370 citing authors

#	Article	IF	Citations
1	Recent Advances in Two-Dimensional Materials beyond Graphene. ACS Nano, 2015, 9, 11509-11539.	14.6	2,069
2	Van der Waals density functional: Self-consistent potential and the nature of the van der Waals bond. Physical Review B, 2007, 76, .	3.2	1,058
3	Porous Graphene as the Ultimate Membrane for Gas Separation. Nano Letters, 2009, 9, 4019-4024.	9.1	850
4	Coupling of Crystal Structure and Magnetism in the Layered, Ferromagnetic Insulator CrI₃. Chemistry of Materials, 2015, 27, 612-620.	6.7	729
5	van der Waals forces in density functional theory: a review of the vdW-DF method. Reports on Progress in Physics, 2015, 78, 066501.	20.1	615
6	Van der Waals density functional: An appropriate exchange functional. Physical Review B, 2010, 81, .	3.2	403
7	A density functional for sparse matter. Journal of Physics Condensed Matter, 2009, 21, 084203.	1.8	363
8	Enhanced Bifunctional Oxygen Catalysis in Strained LaNiO₃ Perovskites. Journal of the American Chemical Society, 2016, 138, 2488-2491.	13.7	310
9	Relationship between local structure and phase transitions of a disordered solid solution. Nature, 2002, 419, 909-911.	27.8	238
10	Magnetic behavior and spin-lattice coupling in cleavable van der Waals layered <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CrCl</mml:mi><mml:mn>3</mml:mn></mml:msub></mm crystals. Physical Review Materials, 2017, 1, .	2.4	216
11	Stacking Interactions and the Twist of DNA. Journal of the American Chemical Society, 2008, 130, 1304-1308.	13.7	181
12	Stacking Interactions and DNA Intercalation. Journal of Physical Chemistry B, 2009, 113, 11166-11172.	2.6	126
13	van der Waals density functionals built upon the electron-gas tradition: Facing the challenge of competing interactions. Journal of Chemical Physics, 2014, 140, 18A539.	3.0	100
14	Oxide chemistry and local structure of PbZrxTi1-xO3 studied by density-functional theory supercell calculations. Physical Review B, 2004, 69, .	3.2	92
15	The effect of octahedral tilting on proton binding sites and transition states in pseudo-cubic perovskite oxides. Journal of Chemical Physics, 2005, 123, 094703.	3.0	89
16	Molecular adsorption on metal surfaces with van der Waals density functionals. Physical Review B, 2012, 85, .	3.2	89
17	Suppression of Defects and Deep Levels Using Isoelectronic Tungsten Substitution in Monolayer MoSe₂. Advanced Functional Materials, 2017, 27, 1603850.	14.9	84
18	A Density Functional Theory Study of the Benzeneâ"Water Complex. Journal of Physical Chemistry A, 2008, 112, 9031-9036.	2.5	79

#	Article	IF	Citations
19	Development of a bond-valence molecular-dynamics model for complex oxides. Physical Review B, 2005, 71, .	3.2	78
20	Reversal of the Lattice Structure in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>SrCoO</mml:mi><mml:mi>x</mml:mi></mml:msub></mml:math>Epitaxial Thin Films Studied by Real-Time Optical Spectroscopy and First-Principles Calculations. Physical Review Letters, 2013, 111, 097401.	7.8	73
21	Facet-Dependent Disorder in Pristine High-Voltage Lithiumâ€“Manganese-Rich Cathode Material. ACS Nano, 2014, 8, 12710-12716.	14.6	71
22	Windowed Carbon Nanotubes for Efficient CO₂ Removal from Natural Gas. Journal of Physical Chemistry Letters, 2012, 3, 3343-3347.	4.6	68
23	Chlorideâ€Reinforced Carbon Nanofiber Host as Effective Polysulfide Traps in Lithiumâ€“Sulfur Batteries. Advanced Science, 2016, 3, 1600175.	11.2	68
24	Tuning Fermi Levels in Intrinsic Antiferromagnetic Topological Insulators MnBi₂Te₄ and MnBi₄Te₇ by Defect Engineering and Chemical Doping. Advanced Functional Materials, 2021, 31, 2006516.	14.9	68
25	Design of tough adhesive from commodity thermoplastics through dynamic crosslinking. Science Advances, 2021, 7, eabk2451.	10.3	66
26	An application of the van der Waals density functional: Hydrogen bonding and stacking interactions between nucleobases. Journal of Chemical Physics, 2008, 128, 204102.	3.0	62
27	Rashba effect in single-layer antimony telluroiodide SbTeI. Physical Review B, 2015, 92, .	3.2	60
28	Discovery of ABO₃ perovskites as thermal barrier coatings through high-throughput first principles calculations. Materials Research Letters, 2019, 7, 145-151.	8.7	60
29	Probing the Local Site Disorder and Distortion in Pyrochlore High-Entropy Oxides. Journal of the American Chemical Society, 2021, 143, 4193-4204.	13.7	60
30	Towards an accurate description of perovskite ferroelectrics: exchange and correlation effects. Scientific Reports, 2017, 7, 43482.	3.3	57
31	Calculated properties of fully hydrogenated single layers of BN,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BC</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> and graphene: Graphane and its BN-containing analogues. Physical Review B, 2009, 80, .	3.2	55
32	Tuning magnetic order in the van der Waals metal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Fe</mml:mi><mml:mn>5</mml:mn></mml:msub></mml:mrow></mml:math> by cobalt substitution. Physical Review Materials, 2020, 4, .	2.4	52
33	Composition dependent intrinsic defect structures in SrTiO₃. Physical Chemistry Chemical Physics, 2014, 16, 15590-15596.	2.8	51
34	Oxygen vacancy diffusion in bulk SrTiO3 from density functional theory calculations. Computational Materials Science, 2016, 118, 309-315.	3.0	48
35	Theoretical and experimental analysis ofH2binding in a prototypical metal-organic framework material. Physical Review B, 2009, 79, .	3.2	47
36	Modern approaches to studying gas adsorption in nanoporous carbons. Journal of Materials Chemistry A, 2013, 1, 9341.	10.3	47

#	ARTICLE	IF	CITATIONS
37	A van der Waals density functional study of adenine on graphene: single-molecular adsorption and overlayer binding. Journal of Physics Condensed Matter, 2011, 23, 135001.	1.8	44
38	Forging Fast Ion Conducting Nanochannels with Swift Heavy Ions: The Correlated Role of Local Electronic and Atomic Structure. Journal of Physical Chemistry C, 2017, 121, 975-981.	3.1	44
39	Antiferromagnetism in the van der Waals layered spin-lozenge semiconductor <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="bold">CrTe</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2017, 95, .	3.2	44
40	Polarization enhancement in short period superlattices via interfacial intermixing. Physical Review B, 2007, 76, .	3.2	39
41	Predicting Cï£¿H/Ï€ Interactions with Nonlocal Density Functional Theory. ChemPhysChem, 2008, 9, 891-895.	2.1	39
42	Computing dispersion interactions in density functional theory. Physics Procedia, 2010, 3, 1417-1430.	1.2	38
43	Predicting the Phase Stability of Multicomponent High-Entropy Compounds. Chemistry of Materials, 2020, 32, 7507-7515.	6.7	37
44	High-temperature magnetostructural transition in van der Waals-layered <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î±</mml:mi><mml:mtext>â^'</mml:mtext><mml:msub><mml:mi mathvariant="bold">CrTe</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> alloys. Physical Review Materials, 2017, 1, .	2.4	37
45	Fractionally Î´-Doped Oxide Superlattices for Higher Carrier Mobilities. Nano Letters, 2012, 12, 4590-4594.	9.1	36
46	Enhanced carrier mobilities in two-dimensional electron gases at III-III/I-V oxide heterostructure interfaces. Physical Review B, 2012, 85, .	3.2	31
47	Enhancing piezoelectricity through polarization-strain coupling in ferroelectric superlattices. Physical Review B, 2009, 79, .	3.2	30
48	Electrical Transition in Isostructural VO2 Thin-Film Heterostructures. Scientific Reports, 2019, 9, 3009.	3.3	28
49	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>J</mml:mi><mml:mi>eff</mml:mi></mml:msub></mml:mrow></mml:math> spin-orbit insulating state close to the cubic limit in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>Ca</mml:mtext><mml:mn>4</mml:mn></mml:msub></mml:math><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>IrO</mml:mtext><mml:m. Physical Review B, 2014, 89, .	3.2	27
50	Supported metal electronic structure: Implications for molecular adsorption. Physical Review B, 2005, 72, .	3.2	26
51	Understanding the interactions between oxygen vacancies atSrTiO3(001) surfaces. Physical Review B, 2014, 90, .	3.2	26
52	Correlating Local Structure with Electrochemical Activity in Li₂MnO₃. Journal of Physical Chemistry C, 2015, 119, 18022-18029.	3.1	26
53	Symmetry-driven phonon chirality and transport in one-dimensional and bulk <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">B</mml:mi><mml:msub><mml:mi mathvariant="normal">a</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math> -derived materials. Physical Review B, 2018, 98, .	3.2	26
54	High Entropy Oxide Relaxor Ferroelectrics. ACS Applied Materials & Interfaces, 2022, 14, 11962-11970.	8.0	26

#	Article	IF	Citations
55	DielectricâEConstantâEnhanced Hall Mobility in Complex Oxides. Advanced Materials, 2012, 24, 3965-3969.	21.0	24
56	Segregation and trapping of oxygen vacancies near the SrTiO3 Î£3 (1 1 2) <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mo mathvariant="bold">[</mml:mo><mml:mover accent="true"><mml:mrow><mml:mn mathvariant="bold">1</mml:mn></mml:mrow><mml:mrow><mml:mo mathvariant="bold">Â¯</mml:mo></mml:mrow></mml:mover><mml:mspace width="0.12em" /><mml:mn mathvariant="bold">1</mml:mn><mml:mspace width="0.12em" /><mml:mn mathvariant="bold">0</mml:	7.9	23
57	Non-conventional mechanism of ferroelectric fatigue via cation migration. Nature Communications, 2019, 10, 3064.	12.8	23
58	Microstructure-Dependent Gas Adsorption: Accurate Predictions of Methane Uptake in Nanoporous Carbons. Journal of Chemical Theory and Computation, 2014, 10, 1-4.	5.3	22
59	Thickness-dependent carrier density at the surface of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mtext>SrTiO</mml:mtext></mml:mrow><mml:mrow><mml:n	3.2	20
60	Effect of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>A</mml:mi></mml:math>-site size difference on polar behavior in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

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73	Perspectives on van der Waals Density Functionals: The Case of TiS₂. Journal of Physical Chemistry A, 2020, 124, 9867-9876.	2.5	13
74	Local Structure of PZT. AIP Conference Proceedings, 2002, , .	0.4	12
75	Hydrogen Adsorption at the Graphene Surface: A vdW-DF Perspective. Physics Procedia, 2012, 34, 34-38.	1.2	11
76	Transparent conducting oxides: A Î´-doped superlattice approach. Scientific Reports, 2014, 4, 6021.	3.3	11
77	Intrinsic interfacial van der Waals monolayers and their effect on the high-temperature superconductor <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>FeSe</mml:mi><mml:mo>/</mml:mo><m Physical Review B, 2019, 100, .	3.2	11
78	Self-assembly of molecular wires on H-terminated Si(100) surfaces driven by London dispersion forces. Physical Review B, 2011, 84, .	3.2	10
79	Spontaneous Formation of Dipolar Metal Nanoclusters. Journal of Physical Chemistry A, 2009, 113, 4134-4137.	2.5	9
80	Symmetry driven control of optical properties in WO₃ films. APL Materials, 2017, 5, 066106.	5.1	9
81	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CrI</mml:mi><mml:mn>3</mml:mn><mml:msub></m revisited with a many-body ab initio theoretical approach. Physical Review Materials, 2021, 5, .	2.4	9
82	Energy level alignment of self-assembled linear chains of benzenediamine on Au(111) from first principles. Physical Review B, 2016, 93, .	3.2	8
83	Noncovalent Interactions in Nanotechnology. , 2017, , 417-451.		8
84	The vdW-DF Family of Nonlocal Exchange-Correlation Functionals. , 2017, , 241-274.		8
85	Oxygen vacancy formation energies in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>PbTiO</mml:mi><mml:mn>3</mml:mn><m superlattice. Physical Review Materials, 2018, 2, .	2.4	8
86	First principles prediction of a morphotropic phase boundary in the Bi(Zn1/2Ti1/2)O3â^'(Bi1/2Sr1/2)(Zn1/2Nb1/2)O3 alloy. Applied Physics Letters, 2011, 98, .	3.3	7
87	Visualization of electronic density. Computer Physics Communications, 2015, 195, 1-13.	7.5	7
88	Surface reconstructions and modified surface states in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">L</mml:mi><mml:msub><mml:mi mathvariant="normal">a</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:msub><mml:mi mathvariant="normal">a</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:mi	2.4	7
89	Extending first principles modeling with crystal chemistry: a bond-valence based classical potential. AIP Conference Proceedings, 2003, , .	0.4	6
90	Oxide-Supported Metal Thin-Film Catalysts: The How and Why. , 2007, , 13-21.		6

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91	...tive behavior of Zn cations in Bi-based perovskites: A comparison of (Bi,Sr)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>ZnNbO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow />	3.2	6
92	Tunable one-dimensional electron gas carrier densities at nanostructured oxide interfaces. Scientific Reports, 2016, 6, 25452.	3.3	6
93	Electronic and magnetic properties of epitaxial SrRhO3 films. Physical Review B, 2017, 95, .	3.2	6
94	Anisotropic antiferromagnetic order in the spin-orbit coupled trigonal-lattice <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ca</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>Co<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow /><mml:mn>6</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2018, 97, .	3.2	6
95	Role of Pairwise Reactions on the Synthesis of Li_{0.3}La_{0.57}TiO₃ and the Resulting Structureâ€“Property Correlations. Inorganic Chemistry, 2021, 60, 14831-14843.	4.0	6
96	Design and Realization of Ohmic and Schottky Interfaces for Oxide Electronics. Small Science, 2022, 2, 2100087.	9.9	6
97	<title>Catalytic behavior at the nanoscale: CO adsorption on Al<formula><inf><roman>2</roman></inf></formula>O<formula><inf><roman>3</roman></inf></formula>-supported Pt clusters</title>. , 2003, , .		5
98	Surface Chemical Reactivity of Ultrathin Pd(111) Films on Ru(0001): Importance of Orbital Symmetry in the Application of the d-Band Model. Journal of Physical Chemistry C, 2015, 119, 23495-23502.	3.1	4
99	Constructing a magnetic handle for antiferromagnetic manganites. Physical Review B, 2016, 93, .	3.2	4
100	Design of a low band gap oxide ferroelectric: Bi 6 Ti 4 O 17. Europhysics Letters, 2011, 94, 37006.	2.0	3
101	Strain effects on the electronic properties in Î´-doped oxide superlattices. Journal Physics D: Applied Physics, 2015, 48, 085303.	2.8	3
102	First Principles Predictions of Van Der Waals Bonded Inorganic Crystal Structures: Test Case, HgCl2. Physics Procedia, 2015, 68, 25-31.	1.2	3
103	Transition Metal Dichalcogenides: Suppression of Defects and Deep Levels Using Isoelectronic Tungsten Substitution in Monolayer MoSe₂ (Adv. Funct. Mater. 19/2017). Advanced Functional Materials, 2017, 27, .	14.9	3
104	Dimensional control of defect dynamics in perovskite oxide superlattices. Physical Review Materials, 2018, 2, .	2.4	3
105	Optical response of BiFeO3 films subjected to uniaxial strain. Physical Review Materials, 2019, 3, .	2.4	3
106	Theoretical studies of Ir₅Th and Ir₅Ce nanoscale precipitates in Ir. Philosophical Magazine, 2014, 94, 991-1000.	1.6	2
107	Mini-review of Electron Density Visualization. Physics Procedia, 2015, 68, 2-6.	1.2	2
108	First principles materials design of novel functional oxides. Journal of Advanced Dielectrics, 2016, 06, 1650011.	2.4	2

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109	Accurate Calculation of CBED Patterns for 4D STEM Using Electron Densities Calculated by Density Functional Theory.. Microscopy and Microanalysis, 2018, 24, 116-117.	0.4	2
110	Unintended consequence of topochemical reduction of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>SrFe</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> to <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>SrFe</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> : Desi	2.4	2
111	Insulating antiferromagnetism in VTe. Physical Review B, 2022, 105, .	3.2	2
112	Thin Films: Understanding Strain-Induced Phase Transformations in BiFeO3 Thin Films (Adv. Sci. 8/2015). Advanced Science, 2015, 2, .	11.2	1
113	Emerging edge states on the surface of the epitaxial semimetal CuMnAs thin film. Applied Physics Letters, 2020, 116, 061603.	3.3	1
114	From Molecules to Solids: A vdW-DF-C09 Case Study of the Mercury Dihalides. Journal of Physical Chemistry A, 2021, 125, 3978-3985.	2.5	1
115	Relating fundamental chemistry and smart materials with DFT calculations. , 0, , .		0
116	Predicting Cï£¿H/Ï€ Interactions with Nonlocal Density Functional Theory. ChemPhysChem, 2008, 9, 1216-1216.	2.1	0
117	Lattice strain effects in graphane and partially-hydrogenated graphene sheets. Materials Research Society Symposia Proceedings, 2009, 1216, 1.	0.1	0
118	Continuum Model of Gas Uptake for Inhomogeneous Fluids. Journal of Physical Chemistry C, 2017, 121, 17625-17632.	3.1	0
119	Investigating Ionic Transport Anisotropy in Oxygen Deficient Lanthanum Cobaltites via STEM and First Principles Theory. Microscopy and Microanalysis, 2017, 23, 1410-1411.	0.4	0