Valentino R Cooper

List of Publications by Year
in descending order

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	Design and Realization of Ohmic and Schottky Interfaces for Oxide Electronics. Small Science, 2022, 2, 2100087.	9.9	6
2	Computationally Accelerated Discovery of High Entropy Pyrochlore Oxides. Chemistry of Materials, 2022, 34, 1459-1472.	6.7	14
3	High Entropy Oxide Relaxor Ferroelectrics. ACS Applied Materials & Interfaces, 2022, 14, 11962-11970.	8.0	26
4	Insulating antiferromagnetism in VTe. Physical Review B, 2022, 105, .	3.2	2
5	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
6	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
7	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
8	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CrI</mml:mi><mml:mn>3</mml:mn> revisited with a many-body ab initio theoretical approach. Physical Review Materials, 2021, 5, .	2.4	9
9	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
10	Design of tough adhesive from commodity thermoplastics through dynamic crosslinking. Science Advances, 2021, 7, eabk2451.	10.3	66
11	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> : Polar	2.4	2
12	Selfâ€Assembled Room Temperature Multiferroic BiFeO₃â€“LiFe₅O₈ Nanocomposites. Advanced Functional Materials, 2020, 30, 1906849.	14.9	14
13	Perspectives on van der Waals Density Functionals: The Case of TiS₂. Journal of Physical Chemistry A, 2020, 124, 9867-9876.	2.5	13
14	Predicting the Phase Stability of Multicomponent High-Entropy Compounds. Chemistry of Materials, 2020, 32, 7507-7515.	6.7	37
15	On the elastic anisotropy of the entropy-stabilized oxide (Mg, Co, Ni, Cu, Zn)O compound. Journal of Applied Physics, 2020, 128, .	2.5	14
16	Emerging edge states on the surface of the epitaxial semimetal CuMnAs thin film. Applied Physics Letters, 2020, 116, 061603.	3.3	1
17	Unexpected crystalline homogeneity from the disordered bond network in <mml:math		

#	ARTICLE	IF	CITATIONS
19	Non-conventional mechanism of ferroelectric fatigue via cation migration. Nature Communications, 2019, 10, 3064.	12.8	23
20	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><mml Physical Review B, 2019, 100, .	3.2	11
21	Discovery of ABO₃ perovskites as thermal barrier coatings through high-throughput first principles calculations. Materials Research Letters, 2019, 7, 145-151.	8.7	60
22	Tuning oxygen electrocatalysis via strain on LaNiO3(001). Physical Chemistry Chemical Physics, 2019, 21, 4738-4745.	2.8	14
23	Electrical Transition in Isostructural VO2 Thin-Film Heterostructures. Scientific Reports, 2019, 9, 3009.	3.3	28
24	Optical response of BiFeO3 films subjected to uniaxial strain. Physical Review Materials, 2019, 3, .	2.4	3
25	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
26	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
27	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 Physical Review B, 2018, 97, .	3.2	6
28	Dimensional control of defect dynamics in perovskite oxide superlattices. Physical Review Materials, 2018, 2, .	2.4	3
29	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></mml superlattice. Physical Review Materials, 2018, 2, .	2.4	8
30	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></ mathvariant="normal">C</mml:mi><mml:msub><mml:mi mathvariant="normal">a</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:mi>Mn</mml:mi><mml:msub><mml:mi	2.4	7
31	Towards an accurate description of perovskite ferroelectrics: exchange and correlation effects. Scientific Reports, 2017, 7, 43482.	3.3	57
32	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
33	Symmetry driven control of optical properties in WO₃ films. APL Materials, 2017, 5, 066106.	5.1	9
34	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
35	Electronic and magnetic properties of epitaxial SrRhO3 films. Physical Review B, 2017, 95, .	3.2	6
36	Continuum Model of Gas Uptake for Inhomogeneous Fluids. Journal of Physical Chemistry C, 2017, 121, 17625-17632.	3.1	0

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37	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
38	Suppression of Defects and Deep Levels Using Isoelectronic Tungsten Substitution in Monolayer MoSe₂. Advanced Functional Materials, 2017, 27, 1603850.	14.9	84
39	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
40	Noncovalent Interactions in Nanotechnology. , 2017, , 417-451.		8
41	The vdW-DF Family of Nonlocal Exchange-Correlation Functionals. , 2017, , 241-274.		8
42	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></mml crystals. Physical Review Materials, 2017, 1, .	2.4	216
43	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 Physical Review Materials, 2017, 1, .	2.4	31
44	First principles materials design of novel functional oxides. Journal of Advanced Dielectrics, 2016, 06, 1650011.	2.4	2
45	Oxygen vacancy diffusion in bulk SrTiO3 from density functional theory calculations. Computational Materials Science, 2016, 118, 309-315.	3.0	48
46	Chlorideâ€Reinforced Carbon Nanofiber Host as Effective Polysulfide Traps in Lithiumâ€“Sulfur Batteries. Advanced Science, 2016, 3, 1600175.	11.2	68
47	Constructing a magnetic handle for antiferromagnetic manganites. Physical Review B, 2016, 93, .	3.2	4
48	Energy level alignment of self-assembled linear chains of benzenediamine on Au(111) from first principles. Physical Review B, 2016, 93, .	3.2	8
49	Tunable one-dimensional electron gas carrier densities at nanostructured oxide interfaces. Scientific Reports, 2016, 6, 25452.	3.3	6
50	Enhanced Bifunctional Oxygen Catalysis in Strained LaNiO₃ Perovskites. Journal of the American Chemical Society, 2016, 138, 2488-2491.	13.7	310
51	Thin Films: Understanding Strain-Induced Phase Transformations in BiFeO3 Thin Films (Adv. Sci. 8/2015). Advanced Science, 2015, 2, .	11.2	1
52	Rashba effect in single-layer antimony telluroiodide SbTeI. Physical Review B, 2015, 92, .	3.2	60
53	Stabilization of weak ferromagnetism by strong magnetic response to epitaxial strain in multiferroic BiFeO3. Scientific Reports, 2015, 5, 12969.	3.3	17
54	Understanding Strainâ€Induced Phase Transformations in BiFeO 3 Thin Films. Advanced Science, 2015, 2, 1500041.	11.2	15

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55	Coupling of Crystal Structure and Magnetism in the Layered, Ferromagnetic Insulator CrI₃. Chemistry of Materials, 2015, 27, 612-620.	6.7	729
56	Strain effects on the electronic properties in Î´-doped oxide superlattices. Journal Physics D: Applied Physics, 2015, 48, 085303.	2.8	3
57	Visualization of electronic density. Computer Physics Communications, 2015, 195, 1-13.	7.5	7
58	Correlating Local Structure with Electrochemical Activity in Li₂MnO₃. Journal of Physical Chemistry C, 2015, 119, 18022-18029.	3.1	26
59	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:mn>	7.9	23
60	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
61	Recent Advances in Two-Dimensional Materials beyond Graphene. ACS Nano, 2015, 9, 11509-11539.	14.6	2,069
62	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
63	Mini-review of Electron Density Visualization. Physics Procedia, 2015, 68, 2-6.	1.2	2
64	First Principles Predictions of Van Der Waals Bonded Inorganic Crystal Structures: Test Case, HgCl2. Physics Procedia, 2015, 68, 25-31.	1.2	3
65	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
66	Understanding the interactions between oxygen vacancies atSrTiO3(001) surfaces. Physical Review B, 2014, 90, .	3.2	26
67	<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:msub><mml:mtext>IrO</mml:mtext><m. Physical Review B, 2014, 89, .	3.2	27
68	Facet-Dependent Disorder in Pristine High-Voltage Lithiumâ€“Manganese-Rich Cathode Material. ACS Nano, 2014, 8, 12710-12716.	14.6	71
69	Theoretical studies of Ir₅Th and Ir₅Ce nanoscale precipitates in Ir. Philosophical Magazine, 2014, 94, 991-1000.	1.6	2
70	Special quasirandom structures to study the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mo>(</mml:mo><mml:msub><mml:mi) Tj ETQq0 0 0 rgBT /Overlock 10 Tf mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>random alloy. Physical Review B, 2014, 90, .	3.2	17
71	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
72	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:r slabs. Physical Review B, 2014, 89, .	3.2	20

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73	Composition dependent intrinsic defect structures in SrTiO₃. Physical Chemistry Chemical Physics, 2014, 16, 15590-15596.	2.8	51
74	Transparent conducting oxides: A Î´-doped superlattice approach. Scientific Reports, 2014, 4, 6021.	3.3	11
75	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
76	Modern approaches to studying gas adsorption in nanoporous carbons. Journal of Materials Chemistry A, 2013, 1, 9341.	10.3	47
77	Enhanced carrier mobilities in two-dimensional electron gases at III-III/I-V oxide heterostructure interfaces. Physical Review B, 2012, 85, .	3.2	31
78	Windowed Carbon Nanotubes for Efficient CO₂ Removal from Natural Gas. Journal of Physical Chemistry Letters, 2012, 3, 3343-3347.	4.6	68
79	La-Driven Morphotrophic Phase Boundary in the Bi(Zn_{1/2}Ti_{1/2})O₃â€“La(Zn_{1/2}Ti_{1/2})O₃â€“PbTiO₃ Solid Solution. Chemistry of Materials, 2012, 24, 4477-4482.	9.7	16
80	Fractionally Î´-Doped Oxide Superlattices for Higher Carrier Mobilities. Nano Letters, 2012, 12, 4590-4594.	9.1	36
81	Hydrogen Adsorption at the Graphene Surface: A vdW-DF Perspective. Physics Procedia, 2012, 34, 34-38.	1.2	11
82	The influence of dispersion interactions on the hydrogen adsorption properties of expanded graphite. Journal of Physics Condensed Matter, 2012, 24, 424205.	1.8	19
83	Molecular adsorption on metal surfaces with van der Waals density functionals. Physical Review B, 2012, 85, .	3.2	89
84	Dielectricâ€Constantâ€Enhanced Hall Mobility in Complex Oxides. Advanced Materials, 2012, 24, 3965-3969.	21.0	24
85	Design of a low band gap oxide ferroelectric: Bi 6 Ti 4 O 17. Europhysics Letters, 2011, 94, 37006.	2.0	3
86	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
87	Relationship between bond stiffness and electrical energy storage capacity in oxides: Density functional calculations for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>h</mml:mi></mml:mrow></mml:math>-La<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow	3.2	14
88	Cooperative 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 /><mml:mrow><mml:mn>6</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>O<mml:math	3.2	6
89	Self-assembly of molecular wires on H-terminated Si(100) surfaces driven by London dispersion forces. Physical Review B, 2011, 84, .	3.2	10
90	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

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91	Computing dispersion interactions in density functional theory. Physics Procedia, 2010, 3, 1417-1430.	1.2	38
92	Polar behavior of the double perovskites<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Bi</mml:mtext><mml:mi>M</mml:mi><mml:msub><mml:mrow><mml:mtext>ZnNbO</mml:mtext>	3.2	15
93	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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109	Oxide-Supported Metal Thin-Film Catalysts: The How and Why. , 2007, , 13-21.		6
110	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
111	Supported metal electronic structure: Implications for molecular adsorption. Physical Review B, 2005, 72, .	3.2	26
112	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
113	Development of a bond-valence molecular-dynamics model for complex oxides. Physical Review B, 2005, 71, .	3.2	78
114	Oxide chemistry and local structure of PbZrxTi1-xO3 studied by density-functional theory supercell calculations. Physical Review B, 2004, 69, .	3.2	92
115	Extending first principles modeling with crystal chemistry: a bond-valence based classical potential. AIP Conference Proceedings, 2003, , .	0.4	6
116	<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
117	Local Structure of PZT. AIP Conference Proceedings, 2002, , .	0.4	12
118	Relationship between local structure and phase transitions of a disordered solid solution. Nature, 2002, 419, 909-911.	27.8	238
119	Relating fundamental chemistry and smart materials with DFT calculations. , 0, , .		0