

Valentino R Cooper

List of Publications by Year in descending order

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119
papers

9,946
citations

93792

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39744

98
g-index

123
all docs

123
docs citations

123
times ranked

17841
citing authors

#	ARTICLE	IF	CITATIONS
19	Non-conventional mechanism of ferroelectric fatigue via cation migration. Nature Communications, 2019, 10, 3064.	5.8	23
20	Intrinsic interfacial van der Waals monolayers and their effect on the high-temperature superconductor FeSe . Physical Review B, 2019, 100, .	1.1	11
21	Discovery of ABO_3 perovskites as thermal barrier coatings through high-throughput first principles calculations. Materials Research Letters, 2019, 7, 145-151.	4.1	60
22	Tuning oxygen electrocatalysis via strain on $\text{LaNiO}_3(001)$. Physical Chemistry Chemical Physics, 2019, 21, 4738-4745.	1.3	14
23	Electrical Transition in Isostructural VO_2 Thin-Film Heterostructures. Scientific Reports, 2019, 9, 3009.	1.6	28
24	Optical response of BiFeO_3 films subjected to uniaxial strain. Physical Review Materials, 2019, 3, .	0.9	3
25	Symmetry driven phonon chirality and transport in one-dimensional and bulk B_3C derived materials. Physical Review B, 2018, 98, .	1.1	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.	0.2	2
27	Anisotropic antiferromagnetic order in the spin-orbit coupled trigonal-lattice CaMn_2P_2 . Physical Review B, 2018, 97, .		
28	Dimensional control of defect dynamics in perovskite oxide superlattices. Physical Review Materials, 2018, 2, .	0.9	3
29	Oxygen vacancy formation energies in PbTiO_3 superlattice. Physical Review Materials, 2018, 2, .		
30	Surface reconstructions and modified surface states in LaMnO_3 . Physical Review B, 2017, 95, .	0.9	7
31	Towards an accurate description of perovskite ferroelectrics: exchange and correlation effects. Scientific Reports, 2017, 7, 43482.	1.6	57
32	Transition Metal Dichalcogenides: Suppression of Defects and Deep Levels Using Isoelectronic Tungsten Substitution in Monolayer MoSe_2 (Adv. Funct. Mater. 19/2017). Advanced Functional Materials, 2017, 27, .	7.8	3
33	Symmetry driven control of optical properties in WO_3 films. APL Materials, 2017, 5, 066106.	2.2	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.	1.5	44
35	Electronic and magnetic properties of epitaxial SrRhO_3 films. Physical Review B, 2017, 95, .	1.1	6
36	Continuum Model of Gas Uptake for Inhomogeneous Fluids. Journal of Physical Chemistry C, 2017, 121, 17625-17632.	1.5	0

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37	Antiferromagnetism in the van der Waals layered spin-lozenge semiconductor CrTe_3 . Physical Review B, 2017, 95, .	1.1	44
38	Suppression of Defects and Deep Levels Using Isoelectronic Tungsten Substitution in Monolayer MoSe_2 . Advanced Functional Materials, 2017, 27, 1603850.	7.8	84
39	Investigating Ionic Transport Anisotropy in Oxygen Deficient Lanthanum Cobaltites via STEM and First Principles Theory. Microscopy and Microanalysis, 2017, 23, 1410-1411.	0.2	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 CrCl_3 crystals. Physical Review Materials, 2017, 1, .	0.9	216
43	High-temperature magnetostructural transition in van der Waals-layered CrI_3 . Physical Review Materials, 2017, 1, .	0.9	216
44	First principles materials design of novel functional oxides. Journal of Advanced Dielectrics, 2016, 06, 1650011.	1.5	2
45	Oxygen vacancy diffusion in bulk SrTiO_3 from density functional theory calculations. Computational Materials Science, 2016, 118, 309-315.	1.4	48
46	Chloride-Reinforced Carbon Nanofiber Host as Effective Polysulfide Traps in Lithium-Sulfur Batteries. Advanced Science, 2016, 3, 1600175.	5.6	68
47	Constructing a magnetic handle for antiferromagnetic manganites. Physical Review B, 2016, 93, .	1.1	4
48	Energy level alignment of self-assembled linear chains of benzenediamine on Au(111) from first principles. Physical Review B, 2016, 93, .	1.1	8
49	Tunable one-dimensional electron gas carrier densities at nanostructured oxide interfaces. Scientific Reports, 2016, 6, 25452.	1.6	6
50	Enhanced Bifunctional Oxygen Catalysis in Strained LaNiO_3 Perovskites. Journal of the American Chemical Society, 2016, 138, 2488-2491.	6.6	310
51	Thin Films: Understanding Strain-Induced Phase Transformations in BiFeO_3 Thin Films (Adv. Sci. 8/2015). Advanced Science, 2015, 2, .	5.6	1
52	Rashba effect in single-layer antimony telluroiodide SbTeI . Physical Review B, 2015, 92, .	1.1	60
53	Stabilization of weak ferromagnetism by strong magnetic response to epitaxial strain in multiferroic BiFeO_3 . Scientific Reports, 2015, 5, 12969.	1.6	17
54	Understanding Strain-Induced Phase Transformations in BiFeO_3 Thin Films. Advanced Science, 2015, 2, 1500041.	5.6	15

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55	Coupling of Crystal Structure and Magnetism in the Layered, Ferromagnetic Insulator CrI ₃ . Chemistry of Materials, 2015, 27, 612-620.	3.2	729
56	Strain effects on the electronic properties in i>Î</i>-doped oxide superlattices. Journal Physics D: Applied Physics, 2015, 48, 085303.	1.3	3
57	Visualization of electronic density. Computer Physics Communications, 2015, 195, 1-13.	3.0	7
58	Correlating Local Structure with Electrochemical Activity in Li ₂ MnO ₃ . Journal of Physical Chemistry C, 2015, 119, 18022-18029.	1.5	26
59	Segregation and trapping of oxygen vacancies near the SrTiO ₃ (1 1 2) surface. Physical Review B, 2014, 89, 114107.	3.8	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.	8.1	615
61	Recent Advances in Two-Dimensional Materials beyond Graphene. ACS Nano, 2015, 9, 11509-11539.	7.3	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.	1.5	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, HgCl ₂ . 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.	1.2	100
66	Understanding the interactions between oxygen vacancies at SrTiO ₃ (001) surfaces. Physical Review B, 2014, 90, .	1.1	26
67	Spin-orbit insulating state close to the cubic limit in Ca ₄ IrO ₁₀ . Physical Review B, 2014, 89, .	1.1	27
68	Facet-Dependent Disorder in Pristine High-Voltage Lithium-Manganese-Rich Cathode Material. ACS Nano, 2014, 8, 12710-12716.	7.3	71
69	Theoretical studies of Ir ₅ Th and Ir ₅ Ce nanoscale precipitates in Ir. Philosophical Magazine, 2014, 94, 991-1000.	0.7	2
70	Special quasirandom structures to study the Ir ₅ Th/Overlock 10 Tf random alloy. Physical Review B, 2014, 90, .	1.1	17
71	Microstructure-Dependent Gas Adsorption: Accurate Predictions of Methane Uptake in Nanoporous Carbons. Journal of Chemical Theory and Computation, 2014, 10, 1-4.	2.3	22
72	Thickness-dependent carrier density at the surface of SrTiO ₃ slabs. Physical Review B, 2014, 89, .	1.1	17

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73	Composition dependent intrinsic defect structures in SrTiO ₃ . Physical Chemistry Chemical Physics, 2014, 16, 15590-15596.	1.3	51
74	Transparent conducting oxides: A $\hat{\Gamma}$ -doped superlattice approach. Scientific Reports, 2014, 4, 6021.	1.6	11
75	Reversal of the Lattice Structure in SrCoO_x Epitaxial Thin Films Studied by Real-Time Optical Spectroscopy and First-Principles Calculations. Physical Review Letters, 2013, 111, 097401.	2.9	73
76	Modern approaches to studying gas adsorption in nanoporous carbons. Journal of Materials Chemistry A, 2013, 1, 9341.	5.2	47
77	Enhanced carrier mobilities in two-dimensional electron gases at III-III/I-V oxide heterostructure interfaces. Physical Review B, 2012, 85, .	1.1	31
78	Windowed Carbon Nanotubes for Efficient CO ₂ Removal from Natural Gas. Journal of Physical Chemistry Letters, 2012, 3, 3343-3347.	2.1	68
79	La-Driven Morphotropic Phase Boundary in the Bi(Zn _{1/2} Ti _{1/2})O ₃ $\hat{\Gamma}$ La(Zn _{1/2} Ti _{1/2})O ₃ $\hat{\Gamma}$ PbTiO ₃ Solid Solution. Chemistry of Materials, 2012, 24, 4477-4482.		
80	Fractionally $\hat{\Gamma}$ -Doped Oxide Superlattices for Higher Carrier Mobilities. Nano Letters, 2012, 12, 4590-4594.	4.5	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.	0.7	19
83	Molecular adsorption on metal surfaces with van der Waals density functionals. Physical Review B, 2012, 85, .	1.1	89
84	Dielectric $\hat{\Gamma}$ Constant $\hat{\Gamma}$ Enhanced Hall Mobility in Complex Oxides. Advanced Materials, 2012, 24, 3965-3969.	11.1	24
85	Design of a low band gap oxide ferroelectric: Bi ₆ Ti ₄ O ₁₇ . Europhysics Letters, 2011, 94, 37006.	0.7	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.	0.7	44
87	Relationship between bond stiffness and electrical energy storage capacity in oxides: Density functional calculations for LaH_3 . LaO	1.1	14
88	Cooperative behavior of Zn cations in Bi-based perovskites: A comparison of (Bi,Sr) O ZnNbO	1.1	6
89	Self-assembly of molecular wires on H-terminated Si(100) surfaces driven by London dispersion forces. Physical Review B, 2011, 84, .	1.1	10
90	First principles prediction of a morphotropic phase boundary in the Bi(Zn _{1/2} Ti _{1/2})O ₃ $\hat{\Gamma}$ (Bi _{1/2} Sr _{1/2})(Zn _{1/2} Nb _{1/2})O ₃ alloy. Applied Physics Letters, 2011, 98, .	1.5	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 $\langle \text{mml:mrow} \langle \text{mml:mtext} \rangle \text{Bi} \langle \text{mml:mi} \rangle \text{M} \langle \text{mml:msub} \langle \text{mml:mrow} \langle \text{mml:mtext} \rangle \text{ZnNbO} \langle \text{mml:mi} \rangle \text{A} \langle \text{mml:mi} \rangle \langle \text{mml:math} \rangle \text{-site size difference on polar behavior in} \langle \text{mml:math} \rangle$	1.1	15
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#	ARTICLE	IF	CITATIONS
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, .	1.1	1,058
111	Supported metal electronic structure: Implications for molecular adsorption. Physical Review B, 2005, 72, .	1.1	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.	1.2	89
113	Development of a bond-valence molecular-dynamics model for complex oxides. Physical Review B, 2005, 71, .	1.1	78
114	Oxide chemistry and local structure of $\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$ studied by density-functional theory supercell calculations. Physical Review B, 2004, 69, .	1.1	92
115	Extending first principles modeling with crystal chemistry: a bond-valence based classical potential. AIP Conference Proceedings, 2003, , .	0.3	6
116	<title>Catalytic behavior at the nanoscale: CO adsorption on Al_2O_3 -supported Pt clusters</title>. , 2003, , .		5
117	Local Structure of PZT. AIP Conference Proceedings, 2002, , .	0.3	12
118	Relationship between local structure and phase transitions of a disordered solid solution. Nature, 2002, 419, 909-911.	13.7	238
119	Relating fundamental chemistry and smart materials with DFT calculations. , 0, , .		0