Anton Van der Ven

List of Publications by Year
in descending order

76 papers	4,614 citations	126907 33 h-index	98798 67 g-index
76 all docs	76 docs citations	76 times ranked	5849 citing authors

#	Article	IF	Citations
1	Potentiometric entropy and operando calorimetric measurements reveal fast charging mechanisms in PNb<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e918" altimg="si211.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>9</mml:mn></mml:mrow></mml:msub></mml:math>O25. Journal of Power Sources, 2022, 520, 230776.	7.8	11
2	Cation Diffusion Facilitated by Antiphase Boundaries in Layered Intercalation Compounds. Chemistry of Materials, 2022, 34, 1889-1896.	6.7	7
3	Pushing the limit of 3d transition metal-based layered oxides that use both cation and anion redox for energy storage. Nature Reviews Materials, 2022, 7, 522-540.	48.7	92
4	Hysteresis in electrochemical systems. , 2022, 1, .		25
5	Order parameters for antiferromagnetic structures: A first-principles study of iridium manganese. Physical Review Materials, 2022, 6, .	2.4	0
6	Delocalized Metalâ€“Oxygen Ï€-Redox Is the Origin of Anomalous Nonhysteretic Capacity in Li-Ion and Na-Ion Cathode Materials. Journal of the American Chemical Society, 2021, 143, 1908-1916.	13.7	62
7	A Two-Step Oxidation Mechanism Controlled by Mn Migration Explains the First-Cycle Activation Behavior of Li2MnO3-Based Li-Excess Materials. Chemistry of Materials, 2021, 33, 1625-1636.	6.7	36
8	MultiShifter: Software to generate structural models of extended two-dimensional defects in 3D and 2D crystals. Computational Materials Science, 2021, 191, 110310.	3.0	7
9	Antiphase boundary migration as a diffusion mechanism in a P3 sodium layered oxide. Physical Review Materials, 2021, 5, .	2.4	5
10	Investigating the electronic origins of the repulsion between substitutional and interstitial solutes in hcp Ti. Physical Review Materials, 2021, 5, .	2.4	1
11	Elucidating the Factors That Cause Cation Diffusion Shutdown in Spinel-Based Electrodes. Chemistry of Materials, 2021, 33, 6421-6432.	6.7	18
12	Role of Electronic Structure in Li Ordering and Chemical Strain in the Fast Charging Wadsleyâ€“Roth Phase PNb₉O₂₅. Chemistry of Materials, 2021, 33, 7755-7766.	6.7	13
13	Comparing crystal structures with symmetry and geometry. Npj Computational Materials, 2021, 7, .	8.7	21
14	Crystallography, thermodynamics and phase transitions in refractory binary alloys. Acta Materialia, 2020, 200, 171-186.	7.9	24
15	Multielectron Redox and Insulator-to-Metal Transition upon Lithium Insertion in the Fast-Charging, Wadsley-Roth Phase PNb₉O₂₅. Chemistry of Materials, 2020, 32, 4553-4563.	6.7	50
16	Multielectron, Cation and Anion Redox in Lithium-Rich Iron Sulfide Cathodes. Journal of the American Chemical Society, 2020, 142, 6737-6749.	13.7	46
17	Linking electronic structure calculations to generalized stacking fault energies in multicomponent alloys. Npj Computational Materials, 2020, 6, .	8.7	19
18	Ordering and Structural Transformations in Layered K_xCrO₂ for K-Ion Batteries. Chemistry of Materials, 2020, 32, 6392-6400.	6.7	13

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19	Mapping skyrmion stability in uniaxial lacunar spinel magnets from first principles. Physical Review B, 2020, 101, .	3.2	14
20	Understanding the interactions between interstitial and substitutional solutes in refractory alloys: The case of Ti-Al-O. Acta Materialia, 2020, 191, 149-157.	7.9	16
21	Rechargeable Alkali-Ion Battery Materials: Theory and Computation. Chemical Reviews, 2020, 120, 6977-7019.	47.7	145
22	Manganese oxidation as the origin of the anomalous capacity of Mn-containing Li-excess cathode materials. Nature Energy, 2019, 4, 639-646.	39.5	164
23	Understanding intercalation compounds for sodium-ion batteries and beyond. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20190020.	3.4	33
24	Revisiting the charge compensation mechanisms in LiNi_{0.8}Co_{0.2â^'y}Al_yO₂ systems. Materials Horizons, 2019, 6, 2112-2123.	12.2	62
25	Phase Stability and Electronic Structure of Tin Sulfide Compounds for Li-ion Batteries. Journal of Physical Chemistry C, 2019, 123, 29086-29095.	3.1	2
26	Toward an Understanding of Deformation Mechanisms in Metallic Lithium and Sodium from First-Principles. Chemistry of Materials, 2019, 31, 8222-8229.	6.7	17
27	Distinction between Intrinsic and X-ray-Induced Oxidized Oxygen States in Li-Rich 3d Layered Oxides and LiAlO₂. Journal of Physical Chemistry C, 2019, 123, 13201-13207.	3.1	33
28	Potassium Ordering and Structural Phase Stability in Layered K_xCoO₂. ACS Applied Energy Materials, 2019, 2, 2629-2636.	5.1	29
29	Fundamental insights about interlayer cation migration in Li-ion electrodes at high states of charge. Journal of Materials Chemistry A, 2019, 7, 11996-12007.	10.3	12
30	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Na</mml:mi><mml:mi>x</mml:mi></mml:m phase stability and hierarchical orderings in the O3/P3 structure family. Physical Review Materials, 2019, 3, .	2.4	38
31	Modeling magnetic evolution and exchange hardening in disordered magnets: The example of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Mn</mml:mi><mml:mrow><mml:mn>1</mml:mn> Heusler alloys. Physical Review Materials, 2019, 3, .	2.4	7
32	Connecting the Simpler Structures to Topologically Close-Packed Phases. Physical Review Letters, 2018, 121, 255701.	7.8	20
33	Phenomenology of chiral Dzyaloshinskii-Moriya interactions in strained materials. Physical Review B, 2018, 98, .	3.2	19
34	Phase Evolution and Degradation Modes of R3Ì…m Li_xNi_{1â€“yâ€“z}Co_yAl_zO₂ Electrodes Cycled Near Complete Delithiation. Chemistry of Materials, 2018, 30, 7545-7574.	6.7	30
35	Machine-learning the configurational energy of multicomponent crystalline solids. Npj Computational Materials, 2018, 4, .	8.7	53
36	Hamiltonians and order parameters for crystals of orientable molecules. Physical Review B, 2018, 98, .	3.2	9

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37	Resolving phase stability in the Ti-O binary with first-principles statistical mechanics methods. Physical Review Materials, 2018, 2, .	2.4	17
38	Crystallography and substitution patterns in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Zr</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mtext>â^’</mml:mtext><mml:mi>Y</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> system. Physical Review Materials, 2018, 2, .	2.4	8
39	First-principles insights on phase stability of titanium interstitial alloys. Physical Review Materials, 2018, 2, .	2.4	10
40	Traction curves for the decohesion of covalent crystals. Applied Physics Letters, 2017, 110, .	3.3	6
41	Role of Crystal Symmetry in the Reversibility of Stacking-Sequence Changes in Layered Intercalation Electrodes. Nano Letters, 2017, 17, 7789-7795.	9.1	76
42	Decohesion models informed by first-principles calculations: The ab initio tensile test. Journal of the Mechanics and Physics of Solids, 2017, 107, 494-508.	4.8	18
43	Narrowing the Gap between Theoretical and Practical Capacities in Liâ€ion Layered Oxide Cathode Materials. Advanced Energy Materials, 2017, 7, 1602888.	19.5	455
44	Symmetry-adapted order parameters and free energies for solids undergoing order-disorder phase transitions. Physical Review B, 2017, 96, .	3.2	33
45	Stability of Prismatic and Octahedral Coordination in Layered Oxides and Sulfides Intercalated with Alkali and Alkaline-Earth Metals. Chemistry of Materials, 2016, 28, 7898-7904.	6.7	82
46	Li intercalation mechanisms in CaTi₅O₁₁, a bronze-B derived compound. Physical Chemistry Chemical Physics, 2016, 18, 32042-32049.	2.8	5
47	Mechanochemical spinodal decomposition: a phenomenological theory of phase transformations in multi-component, crystalline solids. Npj Computational Materials, 2016, 2, .	8.7	52
48	Stacking-Sequence Changes and Na Ordering in Layered Intercalation Materials. Chemistry of Materials, 2016, 28, 8640-8650.	6.7	66
49	Nonequilibrium Pathways during Electrochemical Phase Transformations in Single Crystals Revealed by Dynamic Chemical Imaging at Nanoscale Resolution. Advanced Energy Materials, 2015, 5, 1402040.	19.5	42
50	Mg Intercalation in Layered and Spinel Host Crystal Structures for Mg Batteries. Inorganic Chemistry, 2015, 54, 4394-4402.	4.0	110
51	Factors Contributing to Path Hysteresis of Displacement and Conversion Reactions in Li Ion Batteries. Chemistry of Materials, 2015, 27, 7593-7600.	6.7	27
52	Elucidating the origins of phase transformation hysteresis during electrochemical cycling of Liâ€“Sb electrodes. Journal of Materials Chemistry A, 2015, 3, 18928-18943.	10.3	48
53	Solute embrittlement of SiC. Journal of Applied Physics, 2014, 116, .	2.5	12
54	Ionic Conduction in Cubic Na₃TiP₃O₉N, a Secondary Na-Ion Battery Cathode with Extremely Low Volume Change. Chemistry of Materials, 2014, 26, 3295-3305.	6.7	68

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55	Ab Initio Structure Search and in Situ ⁷Li NMR Studies of Discharge Products in the Liâ€“S Battery System. Journal of the American Chemical Society, 2014, 136, 16368-16377.	13.7	132
56	Low-temperature structural and transport anomalies in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Cu</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">Se</mml:mi></mml:math>. Physical Review B, 2014, 89, .	3.2	54
57	Understanding Li Diffusion in Li-Intercalation Compounds. Accounts of Chemical Research, 2013, 46, 1216-1225.	15.6	476
58	Finite-temperature properties of strongly anharmonic and mechanically unstable crystal phases from first principles. Physical Review B, 2013, 88, .	3.2	138
59	Mesoporous TiO2â€“B microflowers composed of (1 1Ì„ 0) facet-exposed nanosheets for fast reversible lithium-ion storage. Journal of Materials Chemistry A, 2013, 1, 12028.	10.3	60
60	Phase Stability and Transport Mechanisms in Antiperovskite Li₃OCl and Li₃OBr Superionic Conductors. Chemistry of Materials, 2013, 25, 4663-4670.	6.7	204
61	Kinetics of Anatase Electrodes: The Role of Ordering, Anisotropy, and Shape Memory Effects. Chemistry of Materials, 2012, 24, 2894-2898.	6.7	90
62	Configuring pnicogen rings in skutterudites for low phonon conductivity. Physical Review B, 2012, 86, .	3.2	30
63	Thermodynamics of Lithium in TiO₂(B) from First Principles. Chemistry of Materials, 2012, 24, 1568-1574.	6.7	90
64	Tracking lithium transport and electrochemical reactions in nanoparticles. Nature Communications, 2012, 3, 1201.	12.8	254
65	First principles study of competing mechanisms of nondilute Li diffusion in spinel Li<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math>TiS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review B, 2012, 85, .	3.2	67
66	Vacancy mediated substitutional diffusion in binary crystalline solids. Progress in Materials Science, 2010, 55, 61-105.	32.8	95
67	Systematic approach for determination of equilibrium atomic surface structure. Physical Review B, 2010, 82, .	3.2	24
68	Surface atomic order of compound III-V semiconductor alloys at finite temperature. Physical Review B, 2009, 80, .	3.2	10
69	Nondilute diffusion from first principles: Li diffusion in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Li</mml:mtext></mml:mrow><mml:mi>x</mml:mi></mml:msub></mml:mrow></mml:math>Physical Review B, 2008, 78, .	3.2	224
70	Atomic size mismatch strain induced surface reconstructions. Applied Physics Letters, 2008, 92, 062104.	3.3	9
71	Lateral interactions between oxygen atoms adsorbed on platinum (111) by first principles. Molecular Physics, 2004, 102, 273-279.	1.7	33
72	Phase diagram of oxygen adsorbed on platinum (111) by first-principles investigation. Physical Review B, 2004, 70, .	3.2	103

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73	Understanding the Formation Energy of Transition Metal Hydrides. Materials Research Society Symposia Proceedings, 2002, 730, 1.	0.1	1
74	Firstâ€Principles Evidence for Stage Ordering in Li x CoO2. Journal of the Electrochemical Society, 1998, 145, 2149-2155.	2.9	195
75	Thermodynamics of Oxides with Substitutional Disorder: A Microscopic Model and Evaluation of Important Energy Contributions. Journal of the American Ceramic Society, 1998, 81, 517-525.	3.8	32
76	Ab INITIO CALCULATION OF THE LixCoO2 PHASE DIAGRAM. Materials Research Society Symposia Proceedings, 1997, 496, 121.	0.1	5