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	Understanding Li Diffusion in Li-Intercalation Compounds. Accounts of Chemical Research, 2013, 46, 1216-1225.	15.6	476
2	Narrowing the Gap between Theoretical and Practical Capacities in Liâ€ion Layered Oxide Cathode Materials. Advanced Energy Materials, 2017, 7, 1602888.	19.5	455
3	Tracking lithium transport and electrochemical reactions in nanoparticles. Nature Communications, 2012, 3, 1201.	12.8	254
4	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> Physical Review B, 2008, 78, .	3.2	224
5	Phase Stability and Transport Mechanisms in Antiperovskite Li₃OCl and Li₃OBr Superionic Conductors. Chemistry of Materials, 2013, 25, 4663-4670.	6.7	204
6	Firstâ€Principles Evidence for Stage Ordering in Li x CoO2. Journal of the Electrochemical Society, 1998, 145, 2149-2155.	2.9	195
7	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
8	Rechargeable Alkali-Ion Battery Materials: Theory and Computation. Chemical Reviews, 2020, 120, 6977-7019.	47.7	145
9	Finite-temperature properties of strongly anharmonic and mechanically unstable crystal phases from first principles. Physical Review B, 2013, 88, .	3.2	138
10	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
11	Mg Intercalation in Layered and Spinel Host Crystal Structures for Mg Batteries. Inorganic Chemistry, 2015, 54, 4394-4402.	4.0	110
12	Phase diagram of oxygen adsorbed on platinum (111) by first-principles investigation. Physical Review B, 2004, 70, .	3.2	103
13	Vacancy mediated substitutional diffusion in binary crystalline solids. Progress in Materials Science, 2010, 55, 61-105.	32.8	95
14	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
15	Kinetics of Anatase Electrodes: The Role of Ordering, Anisotropy, and Shape Memory Effects. Chemistry of Materials, 2012, 24, 2894-2898.	6.7	90
16	Thermodynamics of Lithium in TiO₂(B) from First Principles. Chemistry of Materials, 2012, 24, 1568-1574.	6.7	90
17	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
18	Role of Crystal Symmetry in the Reversibility of Stacking-Sequence Changes in Layered Intercalation Electrodes. Nano Letters, 2017, 17, 7789-7795.	9.1	76

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19	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
20	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:mn>2</mml:mn></mml:mro	3.2	67
21	Stacking-Sequence Changes and Na Ordering in Layered Intercalation Materials. Chemistry of Materials, 2016, 28, 8640-8650.	6.7	66
22	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
23	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
24	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
25	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
26	Machine-learning the configurational energy of multicomponent crystalline solids. Npj Computational Materials, 2018, 4, .	8.7	53
27	Mechanochemical spinodal decomposition: a phenomenological theory of phase transformations in multi-component, crystalline solids. Npj Computational Materials, 2016, 2, .	8.7	52
28	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
29	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
30	Multielectron, Cation and Anion Redox in Lithium-Rich Iron Sulfide Cathodes. Journal of the American Chemical Society, 2020, 142, 6737-6749.	13.7	46
31	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
32	<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
33	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
34	Lateral interactions between oxygen atoms adsorbed on platinum (111) by first principles. Molecular Physics, 2004, 102, 273-279.	1.7	33
35	Symmetry-adapted order parameters and free energies for solids undergoing order-disorder phase transitions. Physical Review B, 2017, 96, .	3.2	33
36	Understanding intercalation compounds for sodium-ion batteries and beyond. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20190020.	3.4	33

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37	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
38	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
39	Configuring pnicogen rings in skutterudites for low phonon conductivity. Physical Review B, 2012, 86, .	3.2	30
40	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
41	Potassium Ordering and Structural Phase Stability in Layered K_xCoO₂. ACS Applied Energy Materials, 2019, 2, 2629-2636.	5.1	29
42	Factors Contributing to Path Hysteresis of Displacement and Conversion Reactions in Li Ion Batteries. Chemistry of Materials, 2015, 27, 7593-7600.	6.7	27
43	Hysteresis in electrochemical systems. , 2022, 1, .		25
44	Systematic approach for determination of equilibrium atomic surface structure. Physical Review B, 2010, 82, .	3.2	24
45	Crystallography, thermodynamics and phase transitions in refractory binary alloys. Acta Materialia, 2020, 200, 171-186.	7.9	24
46	Comparing crystal structures with symmetry and geometry. Npj Computational Materials, 2021, 7, .	8.7	21
47	Connecting the Simpler Structures to Topologically Close-Packed Phases. Physical Review Letters, 2018, 121, 255701.	7.8	20
48	Phenomenology of chiral Dzyaloshinskii-Moriya interactions in strained materials. Physical Review B, 2018, 98, .	3.2	19
49	Linking electronic structure calculations to generalized stacking fault energies in multicomponent alloys. Npj Computational Materials, 2020, 6, .	8.7	19
50	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
51	Elucidating the Factors That Cause Cation Diffusion Shutdown in Spinel-Based Electrodes. Chemistry of Materials, 2021, 33, 6421-6432.	6.7	18
52	Toward an Understanding of Deformation Mechanisms in Metallic Lithium and Sodium from First-Principles. Chemistry of Materials, 2019, 31, 8222-8229.	6.7	17
53	Resolving phase stability in the Ti-O binary with first-principles statistical mechanics methods. Physical Review Materials, 2018, 2, .	2.4	17
54	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

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55	Mapping skyrmion stability in uniaxial lacunar spinel magnets from first principles. Physical Review B, 2020, 101, .	3.2	14
56	Ordering and Structural Transformations in Layered K_xCrO₂ for K-Ion Batteries. Chemistry of Materials, 2020, 32, 6392-6400.	6.7	13
57	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
58	Solute embrittlement of SiC. Journal of Applied Physics, 2014, 116, .	2.5	12
59	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
60	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
61	Surface atomic order of compound III-V semiconductor alloys at finite temperature. Physical Review B, 2009, 80, .	3.2	10
62	First-principles insights on phase stability of titanium interstitial alloys. Physical Review Materials, 2018, 2, .	2.4	10
63	Atomic size mismatch strain induced surface reconstructions. Applied Physics Letters, 2008, 92, 062104.	3.3	9
64	Hamiltonians and order parameters for crystals of orientable molecules. Physical Review B, 2018, 98, .	3.2	9
65	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
66	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
67	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></mml:mrow></mml:msub></mml:mrow></mml:math> Heusler alloys. Physical Review Materials, 2019, 3, .	2.4	7
68	Cation Diffusion Facilitated by Antiphase Boundaries in Layered Intercalation Compounds. Chemistry of Materials, 2022, 34, 1889-1896.	6.7	7
69	Traction curves for the decohesion of covalent crystals. Applied Physics Letters, 2017, 110, .	3.3	6
70	Ab INITIO CALCULATION OF THE LixCoO2 PHASE DIAGRAM. Materials Research Society Symposia Proceedings, 1997, 496, 121.	0.1	5
71	Li intercalation mechanisms in CaTi₅O₁₁, a bronze-B derived compound. Physical Chemistry Chemical Physics, 2016, 18, 32042-32049.	2.8	5
72	Antiphase boundary migration as a diffusion mechanism in a P3 sodium layered oxide. Physical Review Materials, 2021, 5, .	2.4	5

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73	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
74	Investigating the electronic origins of the repulsion between substitutional and interstitial solutes in hcp Ti. Physical Review Materials, 2021, 5, .	2.4	1
75	Understanding the Formation Energy of Transition Metal Hydrides. Materials Research Society Symposia Proceedings, 2002, 730, 1.	0.1	1
76	Order parameters for antiferromagnetic structures: A first-principles study of iridium manganese. Physical Review Materials, 2022, 6, .	2.4	0