

Anne M Chaka

List of Publications by Year in descending order

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14
papers

697
citations

933447

10
h-index

1058476

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g-index

14
all docs

14
docs citations

14
times ranked

920
citing authors

#	ARTICLE	IF	CITATIONS
1	Effect of the Environment on γ -Al ₂ O ₃ (0001) Surface Structures. <i>Physical Review Letters</i> , 2000, 84, 3650-3653.	7.8	473
2	Ab Initio Thermodynamic Model for Magnesium Carbonates and Hydrates. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7469-7488.	2.5	56
3	Density-functional theory investigation of oxidative corrosion of UO ₂ . <i>Computational and Theoretical Chemistry</i> , 2012, 987, 90-102.	2.5	25
4	Ab Initio Thermodynamics of Hydrated Calcium Carbonates and Calcium Analogues of Magnesium Carbonates: Implications for Carbonate Crystallization Pathways. <i>ACS Earth and Space Chemistry</i> , 2018, 2, 210-224.	2.7	25
5	Ab initio thermodynamics of magnesium carbonates and hydrates in water-saturated supercritical CO ₂ and CO ₂ -rich regions. <i>Chemical Geology</i> , 2016, 434, 1-11.	3.3	23
6	Thermal conductance enhanced via inelastic phonon transport by atomic vacancies at Cu/Si interfaces. <i>Physical Review B</i> , 2020, 102, .	3.2	19
7	Role of Fe(II) Content in Olivine Carbonation in Wet Supercritical CO ₂ . <i>Environmental Science and Technology Letters</i> , 2019, 6, 592-599.	8.7	18
8	Ab initio thermodynamics reveals the nanocomposite structure of ferrihydrite. <i>Communications Chemistry</i> , 2021, 4, .	4.5	17
9	Shell Model for Atomistic Simulation of Lithium Diffusion in Mixed Mn/Ti Oxides. <i>Journal of Physical Chemistry C</i> , 2014, 118, 24231-24239.	3.1	11
10	Quantifying the Impact of Magnesium on the Stability and Water Binding Energy of Hydrated Calcium Carbonates by <i>Ab Initio</i> Thermodynamics. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2908-2923.	2.5	11
11	Ab Initio Thermodynamics and the Relationship between Octahedral Distortion, Lattice Structure, and Proton Substitution Defects in Malachite/Rosasite Group Endmember Pokrovskite Mg ₂ CO ₃ (OH) ₂ . <i>Journal of Physical Chemistry A</i> , 2016, 120, 10181-10195.	2.5	9
12	Thermodynamics of Metal Carbonates and Bicarbonates and Their Hydrates for Mg, Ca, Fe, and Cd Relevant to Mineral Energetics. <i>Journal of Physical Chemistry A</i> , 2020, 124, 1829-1840.	2.5	5
13	Optimization of Thermal Conductance at Interfaces Using Machine Learning Algorithms. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 32590-32597.	8.0	4
14	Effect of interfacial structures on phonon transport across atomically precise Si/Al heterojunctions. <i>Physical Review Materials</i> , 2021, 5, .	2.4	1