

# Anne M Chaka

## List of Publications by Year in descending order

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14  
papers

697  
citations

933447

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