Goldschmidt 2022 Abstract
https://doi.org/10.46427/gold2022.11582

Predicting Silver Chloride Hydration Numbers in High-Temperature Water Vapor with Machine Learning and First-Principles Molecular Simulations

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Hydration numbers of metal complexes in low-density aqueous solutions are required to develop geochemical models for the solubility and transport of ore-forming metals and for the design of emerging supercritical desalination processes. In this study, we investigate the temperature and density dependence of the hydration numbers of silver chloride at 623 K, 673 K, and 713 K and at densities of 10-100 kg/m^3. Experimental literature estimates for the hydration number of AgCl at these conditions are inconclusive, and possibly contradictory, as to the temperature and density trends. To this end, we employ machine-learning-accelerated first-principles molecular simulations to predict AgCl hydration numbers and to elucidate the correct density and temperature dependence. Our molecular simulation results also correctly predict that the hydration number, and thus also the solubility, of AgCl is lower than that of CuCl under the same conditions. Furthermore, our simulations provide atomistic-level detail as to the bond length and angle formed between AgCl and the water complex.

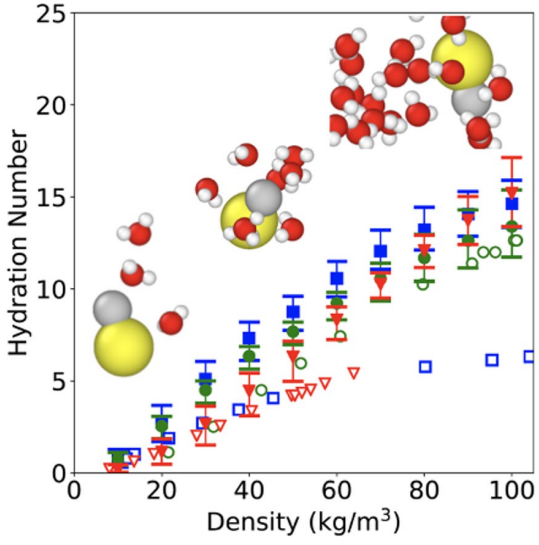

Figure 1: Simulation results (filled symbols) discern between conflicting experimental data (open symbols). Colors correspond to different temperatures: 623 K (blue squares), 673 K (green circles), 723 K (red triangles).