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First Principles Modeling of the Temperature Dependent Ternary Phase Diagram for the Cu-Pd-S System WILLIAM HUHN, MICHAEL WIDOM, Carnegie Mellon University — A method for the prediction of temperature dependent phase diagrams using first principles calculations combined with thermodynamics principles will be discussed. Our method allows us to model the phase diagram without any empirical fitting parameters. Due to the importance of sulfidation when dealing with hydrogen separation using copper palladium membranes, we have chosen as our test case the Cu-Pd-S ternary phase diagram which has been experimentally determined. By applying thermodynamic principles and a simple solid solution model, temperature-dependent features of the Cu-Pd-S system can be explained, specifically solubility ranges for substitutions in select crystalline phases. We have also performed electronic density of states calculations to determine the physical origin of the favorability of select substitutions at T=0K. Work is currently underway to use this method to create phase diagrams where no known experimental results exist, specifically the P-Pd-S system.

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