Goldschmidt 2023 Abstract
https://doi.org/10.7185/gold2023.18752

# Connecting simulations and experiments; a tale of free energies and standard states

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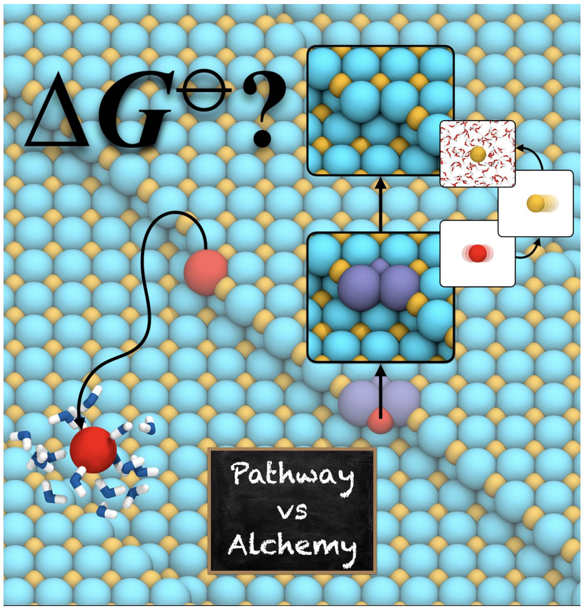

Computer simulations have become routine research tools in most fields of science and engineering, and it is nowadays possible to run atomistic simulations of geochemical systems even on commodity computers. However, even the most accurate simulations may not produce results that are directly comparable with experiments. In fact, one of the less spoken about aspects of thermodynamics is the use of standard reference states for all data, and while the thermodynamic state of experiments is usually well defined, this is not often the case for atomistic simulations. In particular, each simulation may have its own reference state that depends on the system size, temperature, ensemble..., which makes it difficult to compare its results with experiments and other simulations.

In this presentation, I will discuss how we can reconcile the solubilities of minerals computed with different methods, and with experimental values. This requires a careful design of the simulations and the inclusion all the appropriate contributions to refer the results to the thermodynamic standard state. In order to illustrate this approach, I will show our recent results on the calculations of solubilities and surface binding energies for some of the most well-known minerals, *e.g.* halite [1].

**References**

[1] Silvestri, A., Raiteri, P. & Gale, J. D. Obtaining Consistent Free Energies for Ion Binding at Surfaces from Solution: Pathways versus Alchemy for Determining Kink Site Stability. *J Chem Theory Comput* (2022) doi:10.1021/acs.jctc.2c00787.