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Why is Formation Enthalpy Bad for Cluster Expansion Fitting?¹

ANDREW NGUYEN, MARK TRANSTRUM, GUS HART, Brigham Young Univ - Provo — Cluster expansion (CE) allows one to map a relationship between energy and configuration. We often use total energy or formation enthalpy to build a CE model. Since the formation enthalpy is just the transformation of the total energy, one expects that total energy or formation enthalpy would yield similar CE models, i.e., similar errors and a similar number of coefficients. In this study, we are examining the effect of input energies (total energy vs. formation enthalpy) in the cluster expansion formalism. We show that the formation enthalpy generates worse fits, i.e., higher prediction errors and a higher number of coefficients in most cases. We show that correlated noise has little impact on CE models except when that noise is very large. However, the main problem is the transformation of total energy into formation enthalpy which amplifies noise. Thus, we find that it is best to always use the total energy in the fitting. One can always perform the transformation into formation enthalpy after constructing the CE model.

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Andrew Nguyen
Brigham Young Univ - Provo

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