CERE
Center for Energy Resources Engineering

CERE - SEMINAR

Thursday 2 May 2024
09:15 to 10:30 a.m.
Building 229, Room 003
(Light breakfast is served from 9:00, please bring your own coffee/tea)
Online from link in calendar invitation

"Is my solid stable? Reliable thermodynamics for solids from quantum chemistry"

By

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Abstract

Solids play important roles in many technologies, ranging from areas like thermal energy storage to pharmaceuticals. This makes knowledge of their thermodynamic stability crucial if we want to understand their behavior. However, many solids lack these data because it is challenging, expensive and time-consuming to perform accurate measurements of their thermodynamic properties.

In recent decades, developments in electronic structure models based on quantum mechanics (QM) have paved the way for a host of property calculations that have populated large databases. However, the thermodynamic property data contained in these databases are limited or of inadequate accuracy for many applications. Recent atomistic models based on machine-learned QM data appear to provide an attractive avenue towards very fast calculations of thermodynamic properties which could make them attractive for engineers but these methods are more inaccurate than QM.

This seminar will briefly introduce the theory and concepts behind QM-based models of thermodynamic properties of solids and our investigations and work toward robust and fast methodologies for QM-based thermodynamics of solids [1]. The focus of the talk will be on our most recent work on a reaction network-based model for the enthalpy and Gibbs free energy of formation of solids utilizing both atomistic and electronic models, where we obtain excellent performance compared to state-of-the-art methods in this field.

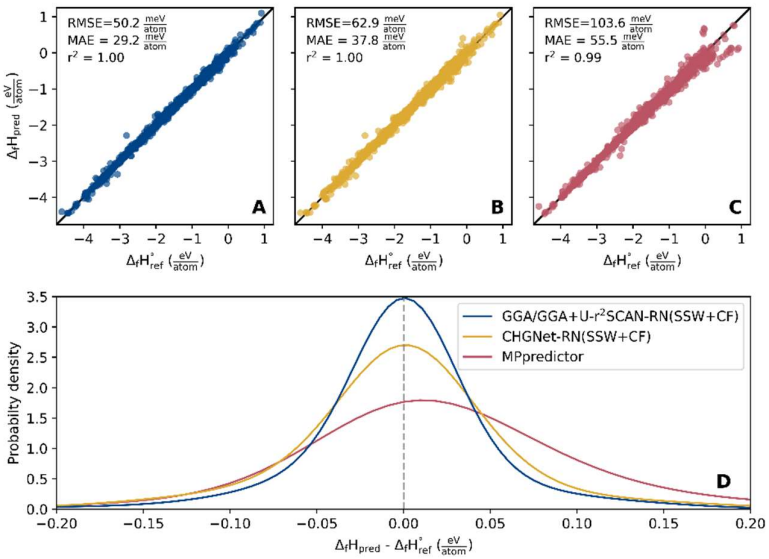

Figure 1 Detailed benchmarks of formation enthalpy predictions at 298.15 K of a selection of methods, for 1545 compounds. (**A**) QM-based reaction network (this work) compared to the experimental reference data. (**B**) QM/ML-based reaction network (this work) compared to the experimental reference data. (**C**) State-of-the-art ML compared to the experimental reference data. (**D**) Kernel density estimate of the distribution of errors in data shown in (A-C). RMSE is the root mean squared error, MAE is the mean absolute error and r^2 is the coefficient of determination.

[1] R. Fromsejer, B. Maribo-Mogensen, G. M. Kontogeorgis, X. Liang, Com. Mat. Sci., vol. 223 (2023), pp. 112152.