

Experimental thermochemistry and theory work together to understand complex mineral phase equilibria under extreme conditions.

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Understanding the stability and reactivity of geochemical, functional and ceramic materials is crucial to optimizing their use and avoiding potentially dangerous situations. The term “stability” is often used in both a thermodynamic and kinetic context. The former means that a given reaction is thermodynamically unfavorable under a given set of conditions (pressure, temperature, composition, atmosphere) and will not occur no matter how long a material is exposed to those conditions. The latter implies that, although a reaction is thermodynamically possible, its rate is negligible under the given conditions and the material, though metastable, is persistent. Experimental thermochemistry (direct measurements of enthalpies, entropies, and free energies of reactions) can distinguish these two cases. Calorimetric measurements of heats of formation and phase transitions and of heat capacities at both cryogenic and high temperatures give values of thermodynamic parameters which can benchmark first principles calculations by DFT and MD methods. Experiment can deal with structurally and compositionally complicated materials including those having complex order-disorder phenomena. Thermochemical measurements also provide much needed data to feed into global data bases and AI analyses. At the same time, such data (both experimental and computational) constrain phase equilibrium calculations using CALPHAD and geochemical approaches. These three strategies (thermochemical experiment, first principles theory, and phase diagram calculation) together provide a solid basis for understanding and predicting phase stability of materials under both terrestrial and planetary extreme conditions of high temperature, high pressure, and radiation fields. New developments in high pressure research in the FORCE initiative at ASU will be summarized.