DOE INFORMAL YEARLY PROGRESS REPORT

Project Title: Energetics of Nanomaterials
Award Number: DE-FG03-01ER15237
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Recent progress

We have investigated the thermodynamics of several nanoscale systems:

Iron oxides: We have completed and published heat capacity and entropy data on goethite, lepidocrocite, and maghemite, as well as measured their heats of formation. We also have enthalpy of formation data for several poorly crystalline nanophase oxides (schwertmannite, ferrihydrite, and epsilon – Fe_2O_3). The next step is to measure thermodynamic properties as a function of surface area for several oxides.

CoO-MgO: Thermochemical data for bulk samples are in press. Heat capacities have been measured for CoO, MgO, and some intermediate samples. Nanosized samples at several compositions are being prepared this summer. Thin films have been prepared and some solution calorimetry done, but additional sample preparation and characterization is needed.

Hydration energetics: Our setups for gas adsorption calorimetry and water immersion calorimetry are being completed. We will test them with known materials (Al_2O_3 , selected zeolites) and then proceed to work on TiO_2 , Fe_2O_3 , and zeolites.

Statement of unexpended funds

We have all our funding for the three-year grant. We anticipate spending it all out in the three years at a rate close to that proposed in the budget.

Publications

"Thermodynamics of Fe Oxides: Part I. Entropy at Standard Temperature and Pressure and Heat Capacity of Goethite ($\alpha\text{-FeOOH}$), Lepidocrocite ($\gamma\text{-FeOOH}$), and Maghemite ($\gamma\text{-Fe}_2\text{O}_3$)", J. Majzlan, B. E. Lang, R. Stevens, A. Navrotsky, B. F. Woodfield, and J. Boerio-Goates, American Mineralogist 88, 846-854 (2003).

"Thermodynamics of Iron Oxides: Part II. Enthalpies of Formation and Relative Stability of Goethite (α -FeOOH), Lepidocrocite (γ -FeOOH), and Maghemite (γ -Fe₂O₃)", J. Majzlan, K. D. Grevel, and A. Navrotsky, *American Mineralogist* 88, 855-859 (2003).

"Thermodynamics of Iron Oxides. III. Enthalpies of Formation and Stability of Ferrihydrite ($\sim$ Fe(OH)₃), Schwertmannite ($\sim$ FeO(OH)_{3/4}(SO₄)_{1/8}), and e-Fe₂O₃", J. Majzlan, A. Navrotsky, and U. Schwertmann, *Geochimica et Cosmochimica Acta* (submitted May 2003).

"Thermodynamics of CoO-MgO Solid Solutions", L. Wang, A. Navrotsky, R. Stevens, B. F. Woodfield, J. Boerio-Goates, *The Journal of Chemical Thermodynamics* (in press).