Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Revealing the Ce gamma-alpha Isostructural Phase Transition YI WANG, LOUISE HECTOR, SHUNLI SHANG, LONG-QING CHEN, ZI-KUI LIU, PENN STATE TEAM, GM COLLABORATION — Since its discovery eighty years ago, the gamma-alpha iso- structural phase transition in cerium has been the subject of numerous theoretical studies. Existing theories, however, yield inaccurate results. Nowhere is this more evident than with the 50-200% disagreement between existing theoretical predictions of the critical point and experiment. We resolve this issue by explicitly incorporating finite temperature mixing of the Ce nonmagnetic and magnetic states into a novel partition function wherein all input quantities are computed with density functional theory. Unique to our approach is the calculation of vibrational properties from phonon theory. The critical behavior of the transition is shown to be controlled by the configurational mixing entropy between the magnetic and nonmagnetic states. Our theoretical framework leads to predicted values of the critical point and equation-of-state that are in remarkably close agreement with experiment and thereby places the Ce gamma-alpha phase transition on a firm theoretical foundation.

Yi Wang

Date submitted: 30 Nov 2008 Electronic form version 1.4