Insight into Structural Phase Transitions from Density Functional Theory

Structural phase transitions caused by high pressure or temperature change are very relevant in materials science [1,2]. The high pressure transitions are essential to understand the interior of planets. Pressure or temperature induced phase transitions can be relevant to understand other phase transitions in strongly correlated systems or molecular crystals.

Phase transitions are important also from the aspect of method development [2,3,4]. Lower level density functionals, LSDA and GGAs all fail to predict the lattice parameters of different polymorphs and the phase transition parameters at the same time. At this time only nonlocal density functionals like HSE and RPA have been proved to resolve the geometry-energy dilemma to some extent in structural phase transitions [5].

In this talk I will report new results from the MGGA_MS family of meta-GGAs and give an insight why this type of meta-GGAs can give a systematic improvement of the geometry and phase transition parameters together [4,6]. I will also present results from the RPA approximation (supported by DoE).

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