Measuring the Performance of Generalized Gradient Approximations in Solids ZACHARY NAULT, A.C. CANCIO, Ball State University — There recently have been a number of generalized gradient approximations (GGA's) developed to address a major limitation of the approach–the inability to model both energies and structural constants at the same time. We examine the performance for bulk systems of four different GGA exchange-correlation (XC) functionals: the PBE functional, best for energy calculations in molecules, the PBEsol functional developed to improve calculations of solid structures, the SOGGA functional developed to improve lattice constant calculations, and the VMT1 functional developed to improve atomization energy calculations without a loss in lattice constant accuracy. These XC functionals are tested on a set of 12 solids composed of metals, semiconductors, ionic metals, and transition metals. The plane-wave DFT code ABINIT was used to calculate the cohesive energy for each solid using each XC approximation. The bulk moduli and lattice constants were determined by fitting to the Murnaghan equation of state. We look particularly into how the use of a pseudopotentail will effect the predictions of each model in comparison to experiment.

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