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New approaches to the prediction of thermodynamic stability of crystal structures[1] JOHANNES VOSS, Materials Research Department, Risoe National Laboratory, DTU; Center for Atomic-Scale Materials Design, Department of Physics, DTU, TEJS VEGGE, Materials Research Department, Risoe National Laboratory, DTU — We present new methods for numerical crystal structure optimization and prediction of structural stability on the basis of density functional theory calculations.[1] Comparison to established approaches to the calculation of lattice free energies differing in numerical complexity and accuracy of the results is provided. We show applications of these methods to complex insulators, semiconductors, and metals, and point out variations of our approaches making them suitable for these different classes of materials. We furthermore briefly outline alternative approaches to the prediction of compound stability avoiding the calculation of free energies. [1] J. Voss and T. Vegge, *to be published* (2007)

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