Materials Genome and Structure Optimization: Structure Prediction in Materials Design

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Materials science is one of the most rapidly growing fields in condensed matter physics and chemistry, and has devoted itself to discover functional materials for various technologically-relevant applications. Recently, novel approaches in computational materials science have led to significant advances in materials design, including high-throughput calculations, data-mining and machine learning[1]. Another increasingly popular technique is *ab-initio* structure prediction, such as the Minima Hopping Method[2], which implements a highly efficient global geometry optimization algorithm to identify thermodynamically stable and metastable compounds. I will illustrate how this method can be used to tackle various materials design challenges from different perspectives, supported by examples of its recent, successful application.

[1] James E. Saal, Scott Kirklin, Muratahan Aykol, Bryce Meredig, and Chris Wolverton, JOM **65**, 15011509 (2013).

[2] Maximilian Amsler and Stefan Goedecker, J. Chem. Phys. **133**, 224104 (2010).