MAR14-2013-000568

Abstract for an Invited Paper
for the MAR14 Meeting of
the American Physical Society

Computational discovery of new structures using the minima hopping method

STEFAN GOEDECKER, University Basel

Theoretical structure prediction methods can find a huge number of possible low energy structures of materials. I will present some basic principles for locating them efficiently and show how these principles are exploited in the minima hopping method. I will next survey some of our applications to various materials. I will present our studies of several hydrogen storage materials for which we found numerous hitherto unknown structures, computer generated silicon allotropes that have promising applications for photovoltaic applications and summarize our search for stable fullerene like structures beyond carbon. I will also address the question of whether theoretically found materials can be synthesized in practice and single out features of the potential energy landscape that facilitate the synthesis.