ISSRNS 2010: Abstracts / Synchrotron Radiation in Natural Science Vol. 9, No. 1 – 2 (2010)

GENETIC ALGORITHMS FOR STRUCTURAL OPTIMIZATION PROBLEMS AT THE NANOSCALE

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Keywords: global optimization, genetic algorithm, nanoscale, scanning tunneling microscopy, cluster, semiconductor surface, nanowire

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In the cluster structure community, global optimization methods are common tools for seeking the structure of molecular and atomic clusters. The large number of local minima of the potential energy surface (PES) of these clusters, and the fact that these local minima proliferate exponentially with the number of atoms in the cluster simply demands the use of fast stochastic methods to find the optimum atomic configuration. Therefore, most of the development work has come from (and mostly stayed within) the cluster structure community. Partly due to wide availability and landmark successes of scanning tunneling microscopy (STM) and other high resolution microscopy techniques, finding the structure of periodically reconstructed semiconductor surfaces was not generally posed as a problem of stochastic optimization until recently, when we have shown that high-index semiconductor surfaces can have a rather large number of local minima with such low surface energies that the identification of the global minimum becomes problematic. We have therefore set out to develop global optimization methods for systems other than clusters, focusing on periodic systems in one- and two- dimensions as such systems currently occupy a central place in the field of nanoscience.

In this talk, we review some of our recent work on global optimization methods (the parallel-tempering Monte Carlo method and the genetic algorithm) and show examples/results from two main problem categories: (a) the two-dimensional problem of determining the atomic configuration of clean semiconductor surfaces, and (b) finding the structure of freestanding nanowires. While focused on mainly on atomic structure, our account will show examples of how these development efforts contributed to elucidating several physical problems and we will attempt to make a case for widespread use of these methods for structural problems in one and two dimensions.