

## **Solving a Class of NP-Hard Optimization Problems**

### **Using Coupled Monte Carlo and Molecular Dynamics Simulations**

**Zig Kuang<sup>1,2</sup>**

<sup>1</sup>Soft Matter Materials Branch (AFRL/RXAS)

Air Force Research Laboratory

2941 Hobson Way, WPAFB, OH 45433

<sup>2</sup>Universal Technology Corporation

1270 North Fairfield Road, Dayton, OH 45432

Email: [zig.kuang@gmail.com](mailto:zig.kuang@gmail.com)

**Abstract.** In computational bio-nano materials design, it is highly demanded to identify the most stable conformer of a macromolecule on nanostructured surfaces. Mathematically, it can be modelled as a global optimization problem in which the potential energy function of the system is the objective function while the coordinates used for representing the structural arrangement of the system are the variables. Due to the combinatorial explosion nature, they are considered as NP-hard optimization problems. In this talk, I will show the mathematical formulation of the optimization problem and a powerful algorithm to obtain optimal solution comparable to experimental result using coupled Monte Carlo and Molecular Dynamics simulations.