A. Project Summary

We propose development and implementation of evolutionary algorithms and their integration with density functional theories to investigate stable conformations of heteronuclear clusters containing metallic elements. Structural, optical, and electronic properties of clusters are of critical importance to chemistry, physics and nanotechnology. This is because clusters offer a unique opportunity to study size-dependent phenomena. Furthermore, clusters form the building blocks of nanocrystals and quasi-crystals. Knowledge of cluster properties can thus be instrumental to the design of nanocrystalline materials.

One fundamental cluster research problem is how to identify stable structures. Interactions between the constituents (atoms, molecules, or ions) of a cluster render a complex potential energy surface (PES). Each minimum on this PES corresponds to a stable cluster structure. A PES may be obtained by either first principle methods such as density functional theory (DFT), or via approximations such as empirical functions. The empirical functions are widely used because they do not treat electrons explicitly and are therefore less computationally expensive. However, unlike the DFT methods, they are not suitable for investigating optical or electronic properties. Moreover, currently empirical potentials are well characterized only for homonuclear clusters.

The number of minima on a PES increases exponentially with the cluster size and finding the global minimum in a PES has been shown to be NP-hard. Monte Carlo (MC) search techniques have been extensively used with the empirically derived PES, although recently several researchers have demonstrated that genetic algorithms (GAs) outperform the MC techniques. Some of our previous work with silicon clusters indicates evolutionary programming (EP)---another widely used evolutionary algorithm---is an even better search algorithm than GAs for this class of optimization problem. We intend to use the powerful search capabilities of an EP in conjunction with the accuracy afforded by a DFT representation of a PES to find stable structures of moderate sized TiC clusters. Nothing of this scale has ever been attempted.

Our specific aims include (i) optimization of reproduction operators and fitness criteria in evolutionary algorithms for searching stable conformations of clusters; (ii) development of a modular evolutionary algorithm program for geometry optimization which can be easily interfaced with several commonly used computer program suites for electronic structure calculations; (iii) optimization of reproduction operators and fitness criteria in evolutionary algorithms for electronic structure calculations; (iv) development of a co-evolutionary algorithm for micro scale (electronic structure) and macro scale (nuclear conformation search). Our objectives, once accomplished, will impact both the fields of evolution programming and physical/theoretical chemistry, and will significantly enhance our ability to characterize clusters and nanoclusters. This is a multi-disciplinary and multi-institutional attempt. A significant component of this proposal is the involvement of graduate and undergraduate students.