DEVELOPMENT OF VIRTUAL TEMPLATES FOR SMALL SEMICONDUCTOR ATOMIC CLUSTERS WITH PRE-DESIGNED OPTO-ELECTRONIC PROPERTIES

Rationale and Problem Formulation

During recent years it was understood that further progress toward orders of magnitude increase in functionality, efficiency and density of active elements of integrated circuits in electronic devises is vital for electronics and technological fields that derive from it (including computing, communication and information storage technologies, source and sensor device development, etc.), and requires novel techniques that would allow manipulations with synthesis of electronic materials at atomic dimensions, rather than at nanoscale. This project is focused on development and applications of self-consistent theoretical and computational methods rooted in the first principles to achieve virtual (i.e., fundamental theory-based, computational) synthesis of small semiconductor atomic clusters with pre-designed electro-optic properties that can be used as templates to guide experimental synthesis of sub-10 nm nanoheterostructure (NHS) units. The clusters' growth parameters (such as the clusters' and their confinement's structure, chemistry and composition) will be computationally manipulated at the atomic scale to ensure that the developed virtual templates exemplify small atomic clusters with optimal electro-optic properties at given sets of synthesis conditions.

Significance of the Proposed Work

Virtual cluster templates developed in the course of this project will provide an unparalleled insight into possible strategies of experimental synthesis of similar atomic clusters with desirable electronic properties at conditions where direct measurements may be difficult to perform and/or interpret, such as cluster synthesis in confinement provided by pores of porous solids, silica and alumina membranes, etc. with pore dimensions in the range of several Angstroms.

Objectives of this project include

- **Theoretical Developments**: (i) estimate accuracy of the Hartree-Fock (HF) -based configuration interaction (CI) and complete active space (CAS) multi configuration self consistent field (MCSCF) methods as applied to computations of the electronic energy level structure of small semiconductor element clusters modeled to reflect their growth in confinement; (ii) formulate a set of tractable correlations between (a) small semiconductor atomic clusters' structure/chemistry/composition and (b) the clusters' electron energy level structure (ELS), optical transition energies (OTE) and spin density distributions (SDDs);
- **Theoretical and Computational Tool Demonstration**: (i) develop algorithms, computation models and codes for virtual (i.e., theory-based, computational) fabrication of small semiconductor element clusters grown in confinement; (ii) apply these models and codes, and existing HF/MCSCF software to virtually synthesize small atomic clusters of Ga, In, Si, Zn with As, P, V, Co and S atoms that would mimic properties of the corresponding clusters grown in confinement; (iii) identify major classes of the template virtual clusters according to their preferential uses for SNHS materials developments.

Novelty of the Proposed Work concerns

- development of theoretical and computational tools to create virtual fabrication templates for small semiconductor atomic clusters grown in confinement and possessing pre-designed opto-electronic properties;
- development of tractable correlations between parameters governing small semiconductor cluster growth in confinement and their major opto-electronic properties.