Virtual Fabrication of 3D Nanoheterostructure Units with Designed Electronic Properties: Development of Theoretical, Modeling and Simulation Fundamentals

Abstract

The objective of the proposed work is to develop theoretical, algorithmic and modeling foundations for virtual (i.e., theory-based, computation-added) synthesis of nanomaterials of designed electronic properties, in particular conductance. This conceptually new approach to electronic materials/device development ensures that the functionality, miniaturization and hardware integration requirements are satisfied at the stage of fabrication at the atomic scale of specific units of integrated circuitry or electronic devices, called nanoheterostructure (NHS) units. Such units can be formed by small quantum dots (QDs) realized in sub-10 nm diameter nanopores of porous silicate materials. Such a NHS unit consists of at least two small QDs, one of which is a crystalline structure formed by guest atoms (such as Ga, As, Al, etc.) deposited in the nanopore, while the other is realized by doping several atomic layers of the confining silicate lattice with the guest atoms. The desired conductance is achieved by manipulations of the NHS composition, structure, and topology of the NHS units during their virtual processing. To enable such manipulations, a fundamental quantum theoretical approach is to be developed in the course of this project on the basis of the Pozhar-Gubbins projection operator method. Implementation (proof of principles) of the theoretical predictions requires some specific algorithm development, computations and simulations that will also be advanced in this project, in synergy with the Hartree-Fock- and density functional theory (DFT)- based computations and simulations, as applied to the above NHS units. The method developed in this project is the first self-consistent attempt at establishing the first-principle theory-based computational methodology of virtual synthesis of electronic nanomaterials. Our research will advance US position toward leadership in the field of virtual synthesis of nanophase materials and will re-inforce its position as an originator of novel, software-based technologies for nanoelectronics.