Project Title: **COMPUTATIONAL AND EXPERIMENTAL FABRICATION OF 3D NANOHETEROSTRUCTURES OF DESIGNED ELECTRONIC PROPERTIES**

Field of Scientific Research: ***Materials Science and Engineering: Theoretical, Computational and Experimental Development of Electronic Nanomaterials***

1. **RATIONALE.** The principles, fabrication methods and device system integration concepts for nanostructures are largely unknown at present. Among other achievements, national priority fields of research have to facilitate breakthrough in nanostructured microprocessor devices to improve the efficacy of computers by a factor of millions, and in integrated nanoprocessor systems capable of collecting, processing and communicating massive amount of data with minimum size, weight and power consumption restrictions. Formidable challenges remain, however, in fundamental understanding of nanoscale system properties before the potential of nanotechnology can be realized. In this project we approach some of these fundamental challenges. Recent progress in fabrication of electronic materials of the characteristic size of several hundred nanometers brought to life new submicron technologies of fabrication of nanoheterostructures for the use in electronic device and intergared circuitry development. Development of experimental nanotechniques, such as scanning near field optical microscopy (SNOM or NSOM) and improved epitaxial growth procedures (MBE and Stranski-Krastanow methods, and improved chemical processing) has lead to fabrication of single quantum dots (QDs) of GaAs, InAs, InP, CuCl, Si, Ge, etc. where up to several thousand electrons are confined to a spatial region of over 10nm in linear dimensions, 2D and 3D ordered arrays of QDs. With this project, we take further important step in this direction bringing the scale down to angstroms and dimensionality to the effective 3D one, and investigating prospects of prediction of electronic properties, modeling and experimental fabrication of 1 to 10nm-sized, 3D nanoheterostructures (NHSs) of desired electronic properties. Conceptually, we plan to approach the problem from a functionality and hardware integration requirements point of view ("functions come first"-concept), rather than via a conventional route, where experimental fabrication of a NHS is attempted before any reliable evaluation of its expected electronic properties. In this project we work on development of theoretical and computational means to relate the key electronic properties (such as conductance) of the simplest NHSs (such as those realized in cylindrical and slit nanopores), on the one hand, and the processing parameters, processed nanosystems' chemistry and composition, and the emerging NHSs' structure, chemistry and composition, on the other hand. If such correlations are known at least for the simplest NHSs, one would have a strategic insight in how to change the processing parameters and the processed nanosystem properties to meet technological requirements applied to the (simplest, in our case) NHS materials, so that functionality and hardware integration requirements can be satisfied (at least, to a significant degree) at the stage of development of nanoscale NHS materials. In particular, we plan to develop theoretical and computational models and molecular simulations to recreate the simplest 3D NHSs of predicted electronic properties at the atomic level by computational "processing" of interfacial "fluids" [such as those composed of Ga, As, Al and P atoms in nanopore confinements of porous silicate carrier matrices], and to use the obtained knowledge and data to develop a strategy of experimental fabrication of samples of the simplest NHSs, and to fabricate experimental samples of 3D NHSs of predicted electronic properties. This will supply an important advance toward development of electronic nanomaterials by design.

2. **OBJECTIVES** of this project development are to:

- estimate fundamental constraints as applied to processing and development of the simplest nanosystems and NHSs in simplest confined geometries; (ii) to merge the quantum statistical mechanical theories (such as the Green function approach merged with the latest functional perturbation theory due to Pozhar and Gubbins) of nonequilibrium phenomena in nanosystems with the Hartree-Fock and density functional theories of the ground state, with the objective to develop a unified and tractable theoretical description of the quantum phenomena (in particular, quantum coherence and role of quantum confinement) in and basic electronic properties (the band width, charge transport coefficients, etc.) of 3D NHS processed at nanoscale; (iii) to use this unified description to reveal correlations between structure, chemistry and composition of the processed nanosystems and processing parameters on the one hand, and the band gaps, electronic charge densities, electron-phonon spectra, electron transports and interconnect conductance, etc., on the other;
- simplify the developed theoretical description, to formulate algorithms and to develop computation and simulation models for virtual fabrication of 3D NHS via virtual nanoscale processing; (ii) to evaluate the developed models by applying them to virtual fabrication of samples of GaAs/AlGaAs- and AlP-based NHSs developed in nanopores of porous silicon and silicate carrier lattices;
- develop experimental techniques of templated synthesis of silicon and silicate porous carrier matrices composed of well-characterized parallel nanopores of up to 30 angstroms in characteristic size (width); (ii) develop experimental techniques of epitaxial growth of GaAs/AlGaAs and AlP-layers confined in the nanopores of the silicon-based carrier matrices; (iii) use the developed experimental techniques in conjunction with the theoretical predictions and computational models to fabricate experimentally samples of GaAs/AlGaAs- and AlP-based NHSs of predicted electronic properties; (iv) use non-destructive characterization techniques and conductance measurements to evaluate experimentally electronic properties of the obtained NHS samples.