Synthesis and Characterization of Nanostructures with Pre-Designed Spin and Charge Transport Properties for Quantum Electronics

B. PROJECT SUMMARY

This project explores applications of quantum mechanics to quantum computing and quantum information processing where **entangled dynamic spin (EDS) states of electrons** of quantum-confined artificial molecules (quantum dots, QDs) or quantum wires are used as quantum bits. This approach potentially meets the major five DiVincenzo criteria for quantum computing and offers all advantages of "solid state"-based hardware operation using external electromagnetic (em) fields and/or electric current. Utilization of EDS states as qubits suggests a cost-effective opportunity to realize quantum computing in a way that is integrable with current electronic technologies. The project will provide a breakthrough in fundamental understanding of evolution of EDS states and their contributions to quantum spin/charge transport properties of the atomic-scale systems imperative to design/operate quantum logic gates using dynamic qubits.

In contrast to existing case-specific, semi-heuristic "quantum" kinetic equation-derived methods and other *ad hoc* "models" that constitute the mainstream of the current theoretical approaches to spin/charge transport and quantum information processing, **the proposed intellectually challenging project is focused on the development of the fundamental, equilibrium two-time temperature Green function (TTGF)-based theoretical and computational methods, to (1) reveal those contributions to the spin/charge transport properties of atomic-scale systems caused by various entangled (E), polarized (P) and otherwise coherent (C) dynamic spin states of electrons, and to (2) identify fundamental mechanisms to support coherence of and manipulate with the EDS states of electrons.** For the first time, the advanced TTGF-based methods of this project will rigorously **account for quantum confinement,** and use the confinement, PC states of electrons, and external em/bias magnetic fields as tools to manipulate EDS states in atomic scale systems. Further progress in experimental preparation of and manipulation with EDS states in the "environment" possessing a variety of types of electron states specific for realistic atomic-scale systems is not possible without theoretical guidance. Theoretical methods of this project will establish, for the first time, a first-principle, self-consistent, and yet tractable methodology that will provide such a guidance.

This methodology will be demonstrated as applied to several exchange-biased systems of small, core-shell Co-CoO and Ni-NiO QDs and nanowires quantum-confined in nanopores of silica and alumina membranes, similar to those synthesized in recent experiments. Ferromagnetic cores (Co or Ni) and antiferromagnetic, semiconductor shells (CoO or NiO, respectively) of such small (few nanometers in dimensions) systems provide conditions favorable for the development of EDS states of electrons. The enhanced contributions of the EPC dynamic electron spin states to the spin/charge transport properties of such systems (below called **intrinsic quantum transport properties**) will be pre-designed by manipulations with the structure and composition of the considered systems, and their confinement. Effects of the em/bias magnetic fields on the intrinsic quantum transport, and thus on the EPC states themselves, will be studied to realize the 1, 2 and 3-qubit quantum logic gates. **A library of virtual (i.e., fundamental theory-based, computational) templates** developed in the project will include digital models of quantum logic gates based on the studied systems.

Advanced theoretical methods developed in the course of this project are crucial for realization of quantum information processing and numerous technologies derived from it and necessary to support further technological growth of the U.S. society. The project's theoretical results and software will significantly contribute to science and education infrastructure, and provide a foundation for joint research with experimentalists focused on synthesis of nanosystems for quantum information processing. Experience and skills gained by the faculty and students involved with the project will advance education and training of the work force mandatory to develop novel quantum information technologies. Extensive dissemination of the project results through the project website, professional and popular publications, lectures and seminars will specifically address talented young people among underrepresented groups, and also business community, to gain their interest, involvement and support.