SPIN/CHARGE TRANSPORT AND ELECTRONIC PROPERTIES OF SMALL "MAGNETIC" QUANTUM DOTS

Increasingly, quantum signal/information processing paradigms are being viewed as a dominant approach to facilitate further advances in communication, information processing and storage technologies, thus providing for the continuing technological growth of the modern society and military infrastructure[1]. Realization of this concept is based upon understanding of structure, quantum spin/charge transport properties and synthesis principles of nanostructure units in quantum confinements that have to be used to enable small QD quantum logic gates and integrated logic-storage units.[2,3] *In contrast to existing case-specific, semi-heuristic "quantum" kinetic equation-derived methods and other "models" that constitute the mainstream of current theoretical approaches, this project develops systematic and fundamental theoretical and computational methods which, in addition to evaluation of possible electron spin/charge correlations, also include quantum confinement into consideration as an important tool to manipulate long-lived coherent/entangled/resonant states of electron spins in quantum dots (QDs) and nanowires synthesized in such confinement.* The project is focused on **(i)** the development of a unique, systematic fundamental theoretical and computational methods specifically designed to predict and verify the key quantum spin/charge transport and magneto-electronic properties of small quantum dots (QDs)/nanowires/artificial molecules in quantum confinement; **(ii)** demonstration of the developed theoretical and computational tools as applied to systems of Co/CoO and Ni/NiO exchange-biased magnetic QDs and nanowires[4] of 3 to 30 nm in characteristic dimensions with pre-designed electron spin/charge transport properties. Outer electrons of semiconductor, antiferromagnetic CoO or NiO "shells" of such QDs and nanowires provide excellent systems to manipulate with, and ferromagnetic states of "cores" of Co or Ni may be used to "store" information at the same time. Such systems exemplify promising sources[4] of coherent/entangled/resonant spin states of electrons that can be used to realize dynamic electronic spin qubits and simultaneous information storage units. The quantum transport properties (such as the conductivity, magnetic and dielectric susceptibility tensors, etc.) of the exchange-biased magnetic QDs/nanowires in ac/dc electromagnetic fields will be predicted by in the framework of a novel (equilibrium) two-time temperature Green function (TTGF)-based method[5,6] [that will refined in the course of this project], and will be related to the QD/nanowire electronic structure, composition and chemistry, and to those of their quantum confinement. Starting from the rigorous quantum Liouville equation, this method reduces the problem of calculation of the transport coefficient to that of the TTGF, which can be predicted analytically, computed and/or deciphered from experimental data. The major advantages of this approach as compared to so-called "quantum" Boltzmann equation-derived methods (that are heuristic quasi-classical adaptations of the classical Boltzmann approach to quantum transport problems), non-equilibrium GF-based, and other "models" include **(i)** systematic, rigorous description of all contributions to coherent/entangled/resonant electron spin motion and the corresponding contributions to the transport coefficients (for which explicit expressions are rigorously derived); **(ii)** rigorous identification of such major contributions to the transport coefficients; and **(iii)** a possibility to use analytical, computational and/or experimental means to obtain equilibrium TTGFs for realistic systems that do not depend on the type of non-equilibrium process. Thus, the major problem of non-equilibrium statistical mechanics, prediction of the transport properties, is reduced to calculation of the equilibrium TTGFs that can be recovered for realistic systems in several practical ways. Special attention will be paid to various components of these coefficients (such as the anomalous, ordinary and intrinsic spin Hall conductivities) caused by reduction of symmetry in effective periodic systems. Availability of realistic analytical and computational predictions for such correlations will provide a strategic insight into physical mechanisms (in particular those involving quantum confinement-supported coherence/entanglement) that shape correlated/polarized/coherent electronic spin states. This insight will help select conditions and QD/quantum confinement parameters that would promote such long-lived coherent/polarized/entangled/resonant electron spin states. To demonstrate the theoretical tools, virtual (i.e., fundamental theory-based, computational) synthesis of model systems of exchange-biased magnetic QDs with pre-designed electron spin/charge transport and magneto-electronic properties is planned.