Zoelitic Materials for Nanoscale Electronics and Quantum Computation

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Proposal goal:

This proposal addresses an avenue toward self-assembled collections of molecular electronic devices, via the synthesis, experimental characterization and theoretical study of zeolitic materials as hosts for single-electron transistors. The aim is a feasibility study wherein open zeolitic frameworks are synthesized to possess single-electron transistor functionality at lattice sites. Individual addressability is obtained through the conducting framework of the zeolitic material: some chains of the framework carry current, others fulfill the role of voltage gates. The individual chains comprising the zeolitic structure are in turn connected to external, macroscopic, metallic electrodes by flexible and functionalized biopolymers such as DNA wires. The result is a self-assembled and chemically contacted dense and vast array of single-electron transistors, with implications for future quantum-computational architectures, nanoelectronics and memory devices.

Research team and objectives:

The proposed work involves an interdisciplinary group of experimental and theoretical physicists and chemists, whose individual contributions will be managed to converge toward the proposal's objective: the fabrication and understanding of chemically contacted, electronically active, zeolitic crystals as hosts for single-electron transistors. Topics addressed by individual researchers include zeolitic materials synthesis and structural characterization, zeolitic material/DNA assembly, contacting and characterization of functionalized DNA wires attached to gold lithographic electrodes, experimental electrical transport characterization of zeolitic material/DNA assemblies, theoretical investigations of collective and single-electron transistor charge transport phenomena in zeolitic materials (in close collaboration with experimental transport measurements), detailed theoretical exploration of the use of zeolitic materials in spin-

based or charge-based quantum computation, and experimental and theoretical comparison of the novel zeolitic single-electron arrays with two-dimensional lithographic equivalents.

Results:

Theoretical results include modeling of zeolitic materials as coupled metallic island arrays, and investigating the application of node-node interactions, as present in the zeolitic framework, toward quantum computation architectures. Charge transport through coupled metallic islands was theoretically studied in three steps. As a first approximation, the motion of an electron through the island array is strongly affected by the appearance of image charges, and these induced charges affect the dynamical properties of the electron. A semi-classical self-consistent calculation of the effective potential and of the dynamically averaged trajectories allows extraction of the quasi-particle effective mass [2]. In a second step, the electrostatic potential for a set of islands and one additional external point charge was calculated numerically in 3D by a relaxation technique on a grid. This microscopic method allows for all charges (external as well as induced), to be determined accurately on the grid. In a third step, an extended Hubbard Hamiltonian was implemented, allowing flexible determination of ground and excited states for various system configurations. The Hubbard model includes many-particle interactions and a mutual capacitance matrix (to deal with island-island interactions, and with voltage probes).

Further developed on the theoretical side were polaron models of relevance to complex molecular chains, such as DSDNA. In these models, the electron interactions with rotational (or twist) degrees of freedom are studied. Such twist modes are active in the stacked chains of DSDNA base pairs, for example, and give rise to strong suppression or enhancement of electron hopping from base to base. This electron - twist phonon coupling can also be derived from microscopic calculations of pi-mediated electronic overlaps between bases. The electron - twist phonon coupling, described as scattering at high temperatures, evolves into bound polarons at lower temperatures. We have incorporated the coupling in a many-body Hamiltonian describing a long chain system, including anharmonicity and non-linear electron-phonon interactions. The resulting states are described by a “twist polaron” with unique dispersion and transport properties [3].

Towards the realization of quantum computation schemes, the exchange interaction between neighboring spins is a promising physical candidate for carrying out quantum gate operations (exchange gates). For the idealized case of vanishing spin-orbit coupling, this interaction is isotropic and the resulting quantum gates can be used for universal quantum computation with appropriate qubit coding. However, for any realistic implementation, spin-orbit coupling leads to anisotropic corrections to the idealized exchange gates. When carrying out a quantum gate by pulsing this interaction, these corrections will not, in general, commute with themselves at different times. This makes the problem of determining the resulting quantum gate nontrivial. To address this, we derived an effective Hamiltonian which produces the same quantum gate as a given pulse, but which does commute with itself at different times. Through a symmetry analysis of this effective Hamiltonian we show that time-symmetric pulsing of the coupling automatically eliminates several undesirable terms. Further, we show that well-chosen pulse shapes produce an effectively isotropic exchange gate which can be used for universal quantum computation [4].

Experimental results encompass functionalization and purification of double stranded DNA (DSDNA) molecules and subsequent measurement of their current-voltage characteristics, and the isolation of vanadium based nanotubes and wires. Strands of λ-phage and D1S80 DSDNA, with unmodified and modified end-groups, were trapped between gold electrodes. Photolithography and electron-beam lithography were utilized for the fabrication of the gold electrodes, on insulating substrates. Current-voltage characteristics, measured at room temperature, indicate that DSDNA molecules support finite electrical conduction when trapped between and contacted by gold electrodes at the molecular ends. The vanadium-based nanotubes and wires were synthesized using hydrothemal techniques, utilizing vanadium salts, amines and alkali chlorides, under conditions propitious to the formation of zeolitic materials. Transmission electron micrographs of these wires show a variety of structures ranging from rods to tubes. Preliminary I-V measurements at room temperature indicate ohmic behavior, whereas the temperature dependence so far points to hopping-dominated transport.

Impact:

This project has relevance to the electrical engineering discipline, present and future. Indeed, nanoelectronics presents one evolutionary pathway from microelectronics, traditionally an electrical engineering topic. Nanoelectronics need nanoscale electrical interconnects, forming the link between the active devices and macroscopic wiring. To bridge this scale gap, we are investigating the feasibility of utilizing biological macromolecules, such as double stranded DNA (DSDNA). In the area of quantum computation, the concept of utilizing zeolitic materials as hosts for coupled quantum dots or single-electron transistors offers a framework for modeling spin-based or charge-based quantum computation schemes.

References

[1] For further information about nanoscience activities at Ohio University, link to **http://www.nqpi.ohiou.edu** or email soghomon@ohio.edu**,** heremans@ohio.edu**,** mccord@ohio.edu**,** ulloa@ohio.edu**, or** bonestee@magnet.fsu.edu
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