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Modal analysis of nano-wires with coupled DFT/FEM calculation

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ABSTRACT

Classical models of bulk solids fail to accurately predict the natural frequency of nano-scale wires. Embedded within classical models is the assumption that for a particular material the electron cloud is, in an average sense, uniform at each material point. This assumption fails at surfaces. Near surfaces, there are broken bonds that may lead to a substantially different strain energy function than in the bulk material. At the macroscale, the contribution to total energy from the surface is small relative to the contribution from the bulk energy, hence it is typically neglected. At the nanoscale, the contribution from surface energy [1] is comparable to the bulk energy, and to obtain correct numerical results, it must be included in a model.

The surface effects are modeled using the Quantum Espresso suite [2,3], a publicly available code that implements density functional theory by way of self-consistent field calculations. To obtain surface energies, a lattice plane is chosen and a super-cell technique is employed. This provides the data for interpolating the surface strain-energy function, which, in turn, provide the material model for a membrane element in an FEM calculation. The wire's modes are computed with an FEM model consisting of bricks accounting for the classical bulk attached at the nodes to surface membranes accounting for the quantum-dominated surfaces.

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