Abstract Submitted
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Simulated Annealing of Nanowire Structures using a Quantum-Based Model[1] ANDREW FRUNEAUX, JEROME BURKI, Sacramento State University — We performed simulations of the equilibrium atomic structures of metallic nanowires based on a classical energy model which includes a short-range (phenomenological hard-core) repulsion, a screened Coulomb potential, and a quantum-mechanics based potential energy that stabilizes longer wires. We simulated cylindrical sodium nanowires with "magic" radii, on order of Angstroms, predicted to be stable by the nanoscale free electron model. The boundary conditions are chosen to simulate a wire connected to bulk contacts. Written in C, our program is based on a Monte-Carlo simulated annealing algorithm and utilizes the double precision SIMD oriented Fast Mersenne Twister (dSFMT) pseudo-random number generator. The simulations performed found that the atoms arrange themselves in multi-shell helical structures.

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Andrew Fruneaux
Sacramento State University

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