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Ab initio investigation of rotaxane-based molecular switches
WENCHANG LU, J. BERNHOLC, North Carolina State University, Raleigh, NC 27695-7518 — A parallel crossbar architecture based on a bistable [2]rotaxane has been achieved experimentally [1]. The rotaxane molecule contains two recognition sites and a macrocyclic ring. Depending on the applied bias, the ring is expected to move from one site to the other and the molecule switches from a high to a low conductance state. We investigate the energetics, forces and quantum transport properties of rotaxane structures using a massively parallel real-space multigrid method. Several stable and metastable configurations are identified and investigated as a function of the applied bias and the current flowing through the molecule. To account for the effects of the current and the open boundary conditions, we use a linear-scaling non-equilibrium Green's function method in a basis of optimized localized orbitals. We discuss current-induced charge redistribution, forces as a function of applied bias, interactions between the ring and the recognition sites, and the I/V characteristics. 1. Luo et al, Chem. Phys. Chem. 3, 519 (2002).

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