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Electrical and structural switching in [2]rotaxane molecular electronic devices YONG-HOON KIM, Korea Institute for Advanced Study, WILLIAM A. GODDARD III, California Institute of Technology — In the effort to identify good candidates of molecular electronics, two-families of redox-controllable mechanically interlocked supramolecular complexes – bistable catenanes and bistable rotaxanes – have attracted much attention. Carrying out large-scale first-principles matrix Green function calculations combined with classical force-field molecular dynamics simulations, we study the charge transport properties of a monolayer of full (including stoppers) bistable rotaxane molecules in their realistic folded conformations. We will discuss (i) the universal nature of the identified switching mechanism in comparison with the [2]catenane device, (ii) the robustness of the switching signal with respect to thermal fluctuations, and (iii) the nature of molecule-electrode barriers that play an important role in inducing a structural switching between the bistable conformations of the molecule, a precondition of observing the electrical switching.

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