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Structure-property relations in electronic switches based on the rotaxane and catenane supramolecular family YONG-HOON KIM, University of Seoul — Mechanically interlocked bistable supramolecular complexes are promising candidates of molecular electronics. Applying a multiscale computational approach combining force-fields molecular mechanics, density-functional theory, and matrix Green's function calculations, we study the structure-property correlations in nanoelectronic switches based on [2]rotaxane and [2]catenane supramolecules. Computational aspects that increase the efficiency of charge transport characteristics calculations while ensuring the numerical accuracy will be also discussed. (This work was supported by the Korea Research Foundation Grant KRF-2007-331-C00077)

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