

Abstract Submitted
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Polymer actuators from first principles NICHOLAS SINGH-MILLER, DAMIAN SCHERLIS¹, NICOLA MARZARI, DMSE, Massachusetts Institute of Technology — We investigate the structure and stability of novel molecular architectures based on the actuation of flexible calixarene hinges and conductive oligothiophenes. When oxidized the oligothiophenes drive the actuation via π -stacking. We investigate from first principles the components of this actuator, paying particular attention to the structure of the hinge, the energetics of π -stacking in charged oligothiophenes, and environmental effects (i.e. solvation and counterions). Since π -stacking occurs in an oxidized state, the latter effects are of particular importance in screening long range Coulomb interactions and the concentration of the charge.

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