Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Polymer actuators from first principles NICHOLAS SINGH-MILLER, DAMIAN SCHERLIS[1], 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 oligothiophens, 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.

[1]Current Address: Departamento de Quimica Inorganica, Analitica y Quimica Fisica, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Ciudad Universitaria, Pab. II, Buenos Aires (C1428EHA) Argentina.

Nicholas Singh-Miller
DMSE, Massachusetts Institute of Technology

Date submitted: 20 Nov 2006 Electronic form version 1.4