Abstract Submitted
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Theory of Molecular Conformational Switching SHASHI KARNA, US Army Research Laboratory — We have investigated stability and current switching as a function of conformational change in tolane molecule by ab initio Hartree-Fock and density functional theory approaches. The planar conformation of the molecule in which the two benzene rings are coplanar is calculated to be more stable than a twisted conformation. The current (I) with respect to the applied external potential (V) increases from minimum to maximum as the two π-rings become planar, suggesting the "ON" and "OFF" mechanism of the molecular switch at planar and perpendicular conformations, respectively.

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