

Abstract Submitted
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Temperature influence on a molecular switching under electric field: quantum transport *ab initio* calculation¹ MAIA VERGNIORY, Donostia International Physics Center, JOSE GRANDINO-ROLDAN, University of Jaen, ARAN GARCÍA-LEKUE, Donostia International Physics Center, LINWANG WANG, Lawrence Berkeley National Laboratory, QUANTUM TRANSPORT TEAM — A molecular transistor based on torsion-angle conformation change driven by gate electric field is designed and studied using *ab initio* calculations. This transistor consists of a SH – C₆H₂F(CH₃)C₆H₂(CH₃)F – SH molecule sandwiched between two Au(111) electrodes, where the interaction between the molecular dipole and a gate voltage induced electric field will cause the molecule to twist along its *c*-axis. This twist changes the quantum conductivity of the molecule. The effect of thermal fluctuation on the molecular conformation is studied, so is the ability of the transistor to shut off its current. The advantages and challenges of using such molecular conformation change as a mechanism for transistor gating are discussed

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