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First-principles study of the spin-polarized electron tunneling in a self-assembled molecular BDT monolayer HAIYING HE, RANJIT PATI, RAVINDRA PANDEY, Michigan Technological University, Houghton, MI, SHASHI P. KARNA, Army Research Laboratory, Aberdeen Proving Ground, MD — Understanding of the "controlled transport of spin-polarized electrons" through a molecular spacer has been an ultimate goal and has attracted much attention in recent years for its potential applications in spin-based molecular electronic devices. In this talk, we will describe the results of the periodic density functional calculations on a self-assembled benzene-1,4-dithiolate (BDT) molecular monolayer. Specifically, we will investigate the effect of spin configurations of the magnetic substrate and atomic magnetic tip on the spin-polarized electron tunneling of the molecular device.

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