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Electron transport through a single chalcogenide $Ni_9Te_6(PEt_3)_8$ cluster[1] GUANGPU LUO, Virginia Tech, VIKAS CHAUHAN, SHIV KHANNA , Virginia Commonwealth University, KYUNGWHA PARK, Virginia Tech — Recently nanoscale chalcogenide-based superatoms have been synthesized in the form of solids and also patterned at the surface of two-dimensional transition metal dichalcogenides as dopants in the laboratory. The superatoms were also theoretically shown to transform from electron donor to acceptor by modifying the ligands. One such superatom consists of a Ni_9Te_6 cluster with a rock-salt structure surrounded by eight PEt_3 ligands which are connected to Ni atoms at the vertices. The superatom has cubic magnetic anisotropy with magnetic anisotropy barrier of 31.55 K in the neutral state. Here we investigate electron transport through an individual $Ni_9Te_6(PEt_3)_8$ cluster in a single-molecule transistor setup, by considering only two charge states within the sequential electron tunneling limit. We calculate current-voltage characteristics without and with an external magnetic field by using the giant spin model with parameter values obtained from density-functional theory and by solving the master equation.

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