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DFT calculations of the charged states of N@C60 and {Fe4} single molecule magnets investigated in tunneling spectroscopy JAVIER NOSSA, FHOKRUL ISLAM, CARLO CANALI, Linnaeus University, Kalmar, Sweden, MARK PEDERSON, Naval Research Laboratory, Washington, USA — For device applications of single molecule magnets (SMMs) in high-density information storage and quantum-state control it is essential that the magnetic properties of the molecules remain stable under the influence of metallic contacts or surface environment. Recent tunneling experiments [1, 2] on N@C60 and {Fe4} SMM have shown that these molecules preserve their magnetic characteristics when they are used as the central island of single-electron transistors. Although quantum spin models have been used extensively to study theoretically tunneling spectroscopy of SMMs, it has been shown recently that the orbital degrees of freedom, which is absent in spin models, can significantly affect the tunneling conductance [3]. In this work we present first-principles calculations of the neutral and charged states of N@C60 and {Fe4} SMMs, and discuss a strategy to include their properties into a theory of quantum transport. We also present results of the magnetic anisotropy for the different charge states of Fe4 and discuss their relevance for experiments [2] in the sequential tunneling and cotunnelling regimes.

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[2]. A.S. Zyazin et al., Nano Lett. 10, 3307 (2010).
[3]. L. Michalak et al., Phys. Rev. Lett. 104, 017202 (2010).

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