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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 environ-
ment. 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.


Md Fhokrul Islam
Linnaeus University

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