The Kondo effect in molecular magnets from first principles
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a magnetic molecule is deposited on a metallic substrate or attached to metallic con-
tacts its magnetic moment may actually be screened by the conduction electrons due
to the Kondo effect. In view of possible applications of molecular magnets such as
nanoscale spintronics and magnetic storage devices, it is important to being able to
predict whether the Kondo effect will take place or not in a given system. Also one
would like to understand in detail how the Kondo effect will take place or not in a given situation
and how it is controlled by the various parameters such as the molecular confor-
mation and the type of substrate. Using a recently developed ab initio approach for
molecular devices [1,2] that explicitly takes into account the strong electronic corre-
lations that give rise to the Kondo effect, we have calculated the electronic structure
and transport properties of different magnetic molecules coupled to nanocontacts [3]
and surfaces [4]. Our calculations shed light on the complex nature of the Kondo
D. Jacob et al., PRB 82, 195115 (2010); [3] M. Karolak et al., PRL 107, 146604