Abstract Submitted
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Many-body electronic structure and Kondo properties of Co-porphyrin molecules on metallic surfaces[1] MURILO TIAGO, Oak Ridge Natl. Laboratory (ORNL), LUIS DIAS DA SILVA, ORNL and University of Tennessee (UT), SERGIO E. ULLOA, Ohio University, FERNANDO REBOREDO, ORNL, ELBIO DAGOTTO, ORNL/UT — Scanning tunneling spectroscopy (STS) studies of the Kondo effect in metallo-organic complexes adsorbed in metallic surfaces has been a thriving area. Despite increasing experimental interest, quantitative theoretical studies of the Kondo properties are rare, largely due to the complex nature of the problem, which requires the accurate treatment of both the molecular electronic structure and the low-energy many-body correlations. In this work, we use a combination of first principles many-body methods (GW) and the numerical renormalization-group (NRG) technique to study the Kondo regime of cobalt-porphyrin compounds adsorbed on a Cu(111) surface [1]. We find the Kondo temperature (T_K) to be highly sensitive to both molecule charging and distance to the surface, which can explain the variations observed in recent STS measurements. We discuss the importance of many-body effects in the molecular electronic structure controlling this phenomenon and suggest scenarios where larger T_K values can be achieved in experiments.

[1] L. Dias da Silva, M. L. Tiago et al. PRB **80** 155443 (2009).

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