



# EINLADUNG zum IFP-SEMINAR

## Many-body physics in quantum impurities and high-spin molecules

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Host: Karsten Held  
Termin: Freitag, 10. Mai 2019, 16:00 Uhr  
Ort: Institut für Festkörperphysik, TU Wien  
Wiedner Hauptstraße 8-10, 1040 Wien  
Seminarraum DB gelb 09 (gelber Bereich, 9. OG)

### Abstract:

Free isolated molecules get structurally as well as electronically remodeled by the presence of an atomic environment, such as a substrate or other molecules. The progresses in the understanding of this complex quantum mechanical influence are so rapid that an “on demand” microscopic control at the atomic scale is no longer considered an unreachable goal. Transition-metal phthalocyanine (TMPc) molecules are characterized by magnetic moments arising from electrons hosted by the d-orbitals at the transition-metal site. The screening from the conduction electrons leads to a, sometimes controllable, Kondo effect [1-3].

In my talk I will present different ways of manipulating the magnetic moment of TMPc, discussing at which stage we currently are in the control of the corresponding many-body correlations. I will show recent scanning tunneling microscopy experiments and density functional theory calculations and supplement the latter with full many-body continuous-time quantum Monte-Carlo calculations. The focus will be put on how the environment not only rearranges electronic levels or lifts orbital degeneracies, but how it can be also used to tune the strength of many-body interactions in single molecules.

[1] J. Kügel, M. Karolak, J. Senkpiel, P.-J. Hsu, G. Sangiovanni and M. Bode Relevance of hybridization and filling of 3d orbitals for the Kondo effect in transition metal Phthalocyanines Nano Letters 14, 3895 (2014)

[2] J. Kügel, M. Karolak, A. Krönlein, J. Senkpiel, P.-J. Hsu, G. Sangiovanni, and M. Bode State identification and tunable Kondo effect on MnPc on Ag(001) Phys. Rev. B 91, 235130 (2015)

[3] J. Kügel, M. Karolak, A. Krönlein, D. Serrate, M. Bode and G. Sangiovanni Reversible magnetic switching of high-spin molecules on a giant Rashba surface Nature npj Quantum Materials 3, 53 (2018)