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EINLADUNG zum IFP-SEMINAR

Spin Cross-over in Metal-organic Complexes: Insights from First-principles Calculations

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Host:	Karsten Held
Termin:	Dienstag, 23 Mai 2017, 10:00 Uhr
Ort:	Institut für Festkörperphysik, TU Wien
	Wiedner Hauptstraße 8-10, 1040 Wien
	Seminarraum DB gelb 09 (gelber Bereich, 9. OG)
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Molecules or molecular assemblies containing transition metal centers connected by organic ligands, are in focus of attention due to their appealing perspective of being used in information processing. One of most spectacular examples of molecular bistability is the spin-crossover phenomena. The essence of the spin-crossover (SCO) phenomena [1,2,3] is that molecular species containing an octahedral coordinated or tetrahedral coordinated transition metal ion with $3d^n$ ($4 <= n <= 7$) electronic configuration may show a crossover between a low-spin (LS) and high-spin (HS) state. Crossover may be induced by variation of temperature, pressure, magnetic field, strain, introduction of guest molecule etc.

To be useful as devices, it is desirable to make the SCO phenomena cooperative implying spin transition rather than spin crossover, which may happen with associated hysteresis effect. Employing density functional theory (DFT) based calculations, along with model study, we perform a computational investigation to unravel the intricate spin-crossover transitions that have been observed in coordination polymers [4] and its designing in hybrid perovskites [5].

[1] Tanusri Saha-Dasgupta and Peter M Oppeneer, MRS Bulletin, **39**, 614 (2014).
[2] Pablo Maldonado, Sudipta Kanungo, Tanusri Saha-Dasgupta, and Peter M. Oppeneer, Phys. Rev. B (Rapid) **88**, 020408 (2013).
[3] Soumyajit Sarkar, Kartick Tarafder, Peter M. Oppeneer and Tanusri Saha-Dasgupta, J. Mater. Chem. **21**, 13832 (2011).
[4] K. Tarafder, S. Kanungo, P. M. Oppeneer, and T. Saha-Dasgupta, Phys. Rev. Lett. **109**, 077203 (2012).
[5] H Banerjee, S Chakraborty, T Saha-Dasgupta, Chemistry of Materials **28**, 8379 (2016).