# Control of magnetism in transition metal doped oxides

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Transition metal doping of oxides may or may not make the system ferromagnetic. Both theory and experiment suffer of poor reproducibility [1,2,3]. In this talk, I will outline the typical pitfalls of first principles calculations for transition metal doped oxides [1]. At dilute defect concentrations, long-range magnetic interactions need to be mediated by charge carriers in the oxide host, but conventional density-functionals fail to correctly describe carrier localization properties. I will discuss systematic correction schemes that correctly capture the carrier localization properties for various magnetic semiconductor/oxide systems [4-6]. Finally, I will discuss strategies how to control the onset of ferromagnetism by external stimuli, such as electrical gating and mechanical strain [7].

References

[1] A. Zunger, S. Lany, H. Raebiger, Physics 3, 53 (2010).
[2] L. M. C. Pereira, J. Phys. D 50, 393002 (2017).
[3] J. M. D. Coey, Nature materials 18, 652 (2019).
[4] H. Raebiger, S. Lany, A. Zunger, Phys. Rev. Lett. 101, 027203 (2008).
[5] S. Bae, H. Raebiger, Phys. Rev. B 94, 241115R (2016).
[6] K. Ichihashi, H. Shinya, H. Raebiger, Appl. Phys. Expr. 13, 021002 (2020).
[7] H. Raebiger, S. Bae, C. Echeverria-Arrondo, A. Ayuela, Phys. Rev. Mater. 2, 024402 (2018).