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TÉMA

Beyond-DFT corrections for quantum transport simulations

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The theoretical understanding of the atomic and electronic structure, and of the resulting electron transport phenomena at the atomic scale is essential for the design of new nanoscale devices. While standard density functional theory (DFT) based quantum transport simulations can usually explain experiments on a qualitative level, the quantitative agreement is rather poor due to the often incorrectly predicted energy level alignment and charge transfer at metal/molecule interfaces. In this talk we will first give an overview of the limitations of DFT, and then present the required corrections implemented in the Smeagol quantum transport code [1,2] to improve the agreement with experiment. These are based on the self-interaction correction [3], constrained DFT combined with a scissor operator [4-6], as well as a single impurity Anderson model and the dynamical mean field theory (DFMT) [7-8] for magnetic systems.

[1] A. R. Rocha et al., Phys. Rev. B 73, 085414 (2006).
[2] I. Rungger et al., Phys. Rev. B 78, 035407 (2008).
[3] A. M. Souza et al., Nanoscale 6, 14495 (2014).
[4] A. M. Souza et al.Sanvito, Phys. Rev. B 88, 165112 (2013).
[5] A. Droghetti et al., Nature Comm. 7, 12668 (2016).
[6] A. V. Rudnev et al., Science Adv. 3, e1602297 (2017).
[7] A. Droghetti and I. Rungger, Phys. Rev. B 95, 085131 (2017).
[8] L. Chioncel et al., Phys. Rev. B 92, 054431 (2015).

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