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### **Self-interaction errors in density functional calculations of electronic transport**

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All density functional (DFT) calculations of single-molecule transport to date have used continuous exchange-correlation approximations, such as the local density approximation (LDA) or the generalized gradient approximation (GGA). These usually provide a good description of metallic systems, but fail in predicting the correct I-V curve for molecules weakly coupled to the current/voltage probes. Most of the problem can be attributed to the lack of the derivative discontinuity of the DFT potential in local approximations. These in fact continuously connect the orbital levels for different integer occupations, leading to qualitative errors such as the erroneous prediction of the dissociation of heteronuclear molecules into fractionally charged ions. In this talk I will first describe the typical errors arising from neglecting the derivative discontinuity in transport calculations [1], namely the erroneous prediction of metallic transport for insulating molecules. Then I will present a simple and computationally undemanding atomic self-interaction correction scheme for transport. This preserves the computational and conceptual simplicity of standard LDA, and nevertheless re-introduces part of the derivative discontinuity. The method is implemented in our quantum transport code Smeagol [2] ([www.smeagol.tcd.ie](http://www.smeagol.tcd.ie)) and several examples will be given.

[1] C.Toher, A.Filippetti, S.Sanvito, and K.Burke, Phys. Rev. Lett. 95, 146402, (2005).

[2] A.R.Rocha, V.M.Garcia Suarez, S.W.Bailey, C.J.Lambert, J.Ferrer, and S.Sanvito, cond-mat/0510083