Title : **(in English)** *Re-using model results to determine materials properties: connector theory approach*		
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Research Area : *Condensed Matter Physics, (Mathematical Physics)*		
Methods: *static and time-dependent Density Functional Theory, Green's functions*		

PhD track subject :

Most simple approximations to Density Functional Theory (DFT) use, in one way or the other, pre-existing results that were obtained by other methods for a model, the homogeneous electron gas. This "recycling" of model knowledge may explain the efficiency and huge success of DFT. The present project is part of a research line that turns the idea into a very general and in principle exact approach called connector theory (COT) [1,2]. Specifically, we will use COT to develop new approximations for electronic excitations and spectroscopy. The work is analytical and numerical.
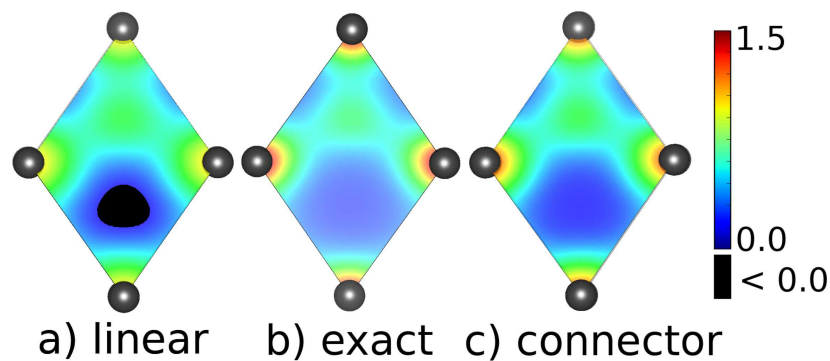

Fig. 1: Charge density of silicon, result of perturbation theory (a) compared to full calculation (b) and using the same approximation as in (a) but in conjunction with COT (c). The use of COT leads to significant improvement.

References :

[1] M. Panholzer, M. Gatti, L. Reining, Phys. Rev. Lett. 120, 166402 (2018)
[2]A. Aouina, M. Gatti, L. Reining, Faraday Discussions 224, 27 (2020)