Local correlation methods for molecules and solids

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During the last two decades local correlation methods have evolved to an efficient computational tool to treat extended molecular systems and also periodic infinte systems like solids[1] beyond the realm of density functional theory. In the first part of my contribution I will discuss so called pair approximation in local coupled cluster theory: In the context of local coupled cluster theory individual pairs of occupied orbitals are usually discriminated on the basis of the inter orbital distance, or the size of the MP2 estimate of the pair energy. Only strong pairs are treated at the full coupled cluster level, while weak pairs are treated just at the MP2 level. Yet MP2 might be problematic for certain situations, for example π-stacking interactions. It will be shown that an approach based on ring-CCD including diagrams up to third order is clearly superior to MP2 and still computationally cheap.

In the second part of my contribution I will discuss recent advances in the correlated treatment of solids. First results of the recently implemented periodic local MP2 program based on orbital specific virtuals will be presented.

[1] C. Pisani, M. Schütz, S. Casassa, D. Usvyat, L. Maschio, M. Lorenz, and A. Erba, *Phys. Chem. Chem. Phys*, 14:7615, 2012.