Quantum Embedding Theories

A talk by Fred Manby

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LOCATION: Seminar Room DB gelb 09, TU Wien, "Freihaus"- building, 9th floor, "yellow"

Issues of accuracy in density functional theory can be addressed by making accurate methods (like coupled-cluster theory) more efficient; or by making density-functional approximations more accurate. Efforts in both directions are underway in our group, and in many groups around the world; but in this talk I will focus on a third possibility, namely the development of quantum-mechnical multiscale models that enable the use of a high-accuracy method in a small, physically important region coupled to density-functional theory (or other low-cost methods) to describe the molecular environment.