PHYSIKALISCHES KOLLOQUIUM

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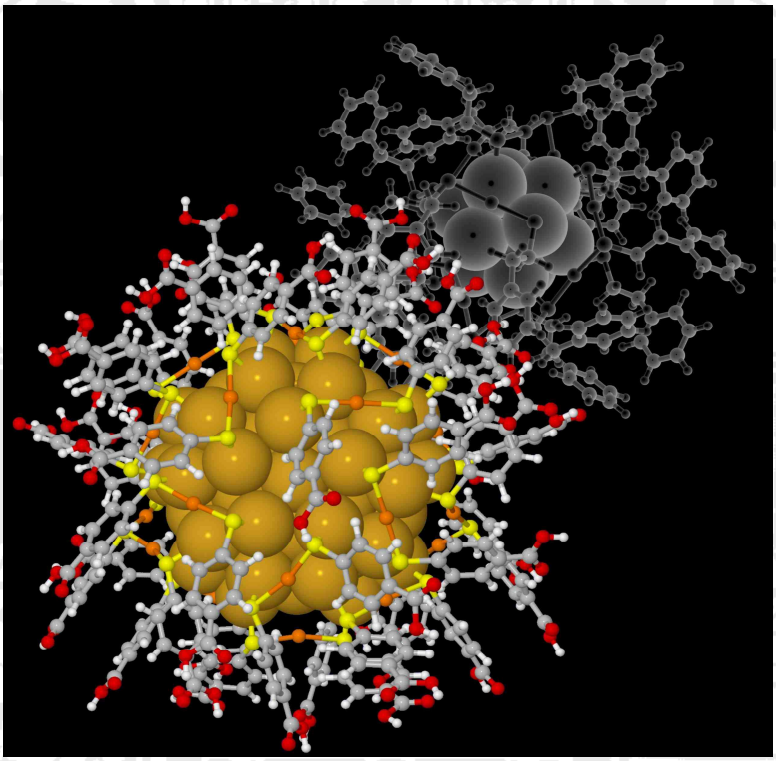
IM GROßEN HÖRSAAL



APPLICATION OF DENSITY FUNCTIONAL THEORY TO NANOPARTICLES: MANY-BODY EFFECTS FROM SEEMINGLY NONINTERACTING ELECTRONS

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Density functional theory (DFT) is the de facto standard for calculations of the electronic structure of matter due to its favorable cost to accuracy ratio. It is applicable for finite systems like molecules in the gas phase as well as for infinite systems like solids. Time dependent DFT extends this ground state theory also to the range of excited states. The possibilities and limitations of DFT in principle and in practice are discussed. Some examples of our recent work are presented that are related to metal clusters in different environments. It is shown, that the effective single-particle picture can explain many properties of rather complicated systems but breaks down for the simplest clusters when the wrong question is asked.