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Pushing the Envelope Beyond Standard Density Functional Theory for Simulations of Zero Emission Energy Materials

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This talk will provide an update into two quantum mechanics techniques that my group has been developing over the past 20 years: embedded correlated wavefunction theory and orbital-free density functional theory (OF-DFT). The first technique locally refines the electronic structure beyond standard DFT and can be used to study localized phenomena such as charge transfer or excited states where standard DFT approximations are inaccurate. The correlated wavefunction methods treat electron exchange exactly and electron correlation systematically, leading to very accurate predictions. The embedding potential is derived from optimized effective potential theory and is formally unique and exact. Examples will be given from our recent efforts to design plasmonic nanocatalysts that can use visible light to break chemical bonds that conventionally use energy from fossil fuels to do so. The second technique is aimed at much larger sample sizes, in order to compute properties involving larger-length-scale features. OF-DFT solves directly for the electron density – no wavefunctions – and therefore can be made (quasi)linear scaling with a small prefactor. Because of the lack of wavefunctions, electron kinetic energy must be evaluated using a density functional; we have developed many over the years that obey exact limits for certain classes of materials. Here we will give examples of our work studying properties of (i) complex lightweight metal alloys, which could improve fuel efficiency if used in vehicle construction, and (ii) liquid metals under consideration as first wall materials in fusion reactors.