SPECIAL CHEMISTRY SEMINAR

Unconventional Quantum Mechanics Methods for Design of Materials for Sustainable Energy Technologies

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and

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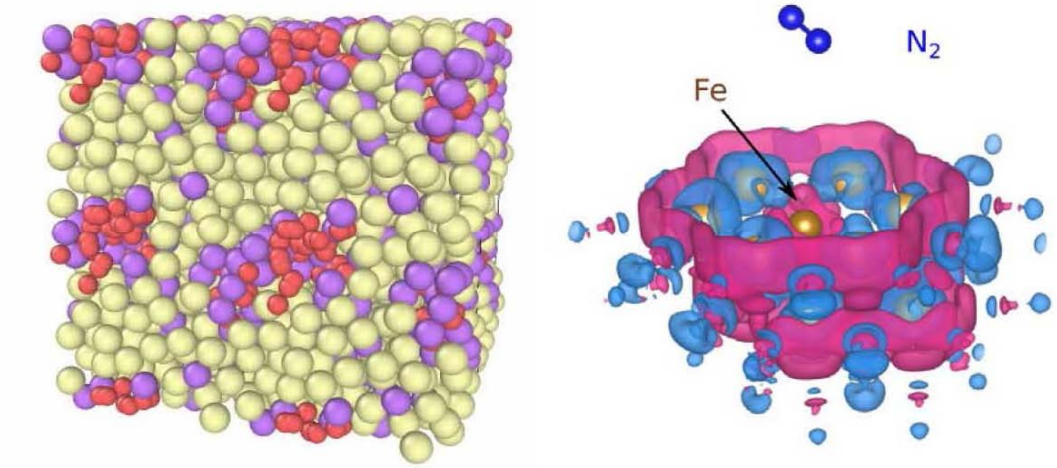
Two quantum mechanics methods developed in my research group over the past two-plus decades, orbital-free density functional theory (OFDFT) and embedded correlated wavefunction (ECW) theory, are useful alternatives to conventional Kohn-Sham (KS) DFT for studying certain materials and phenomena of relevance for sustainable energy technologies. I will introduce these two methods in the context of these applications, emphasizing both their advantages and limitations. We are using OFDFT (and KSDFT) molecular dynamics simulations to evaluate first wall material candidates for fusion reactors and ECW theory to characterize plasmon-induced catalysis by visible-light-illuminated metal nanoparticles. Insights from these studies suggest optimal metal alloys both for fusion reactor walls and for photocatalysis.



Monday, October 7, 2019
3:00 p.m.
SOS B4
(Social Sciences Building next to VKC)

The Scientific Community is Invited