

Abstract Submitted  
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**Applications of DFT to Lanthanides and Precious Metal Complexes** ALEX BALBOA, MARGARET HURLEY, US Army, AMANDA JENKINS, Ask Incorporated, NONE COLLABORATION, NONE COLLABORATION — Density functional theory is widely used for computational characterization of novel materials. While study of materials containing the lighter elements is commonplace, the application of these methods to the bottom of the periodic table, including the lanthanides and the heavier precious metals such as Osmium, requires careful validation. Here we present results of recent quantum mechanical studies to characterize Lanthanide/Graphene Materials and assess the suitability of DFT for these systems. Additionally, we will present recent work on similar application of DFT to characterize Os bipyridine complexes.

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