Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Computational Modeling of Actinide Complexes Pertinent to Environment KRISHNAN BALASUBRAMANIAN, Lawrence Livermore National Lab — We discuss computational projects relevant to actinide separation, complexes and the possibility of actinide sequestration by engineered mesoporous materials We have carried out computational studies on a number of actinide complexes in aqueous solution; as such complexes are of considerable importance in our understanding of behavior of actinide species in the environment and high level nuclear waste, especially experimental-theoretical collaboration on curium (III) complexes with multi-dentate ligands with Nitsche and coworkers at LBNL. Cu(III) complexes with phosphonic acid (PPA) were studied for assessing relative binding strengths of the two ligands with varying pH. Possible isomers of CmH2PPA2+ and CmHPPA+ complexes were computed both in the gas phase and aqueous solution and the results of spectra and geometry will be discussed. The effects of the aqueous solvent in the configuration preferences of CmH2PPA2+ and We have also studied aqueous complexes of U(VI), Np(VI) and Pu(VI) with OH-. We will discuss the results of out extensive *ab initio* computations on the equilibrium structure, infrared spectra, and bonding characteristics of a variety of hydrated NpO2(CO3)m^{q-} complexes by considering the solvent as a polarizable dielectric continuum as well as the corresponding anhydrate complexes in the gas-phase. The work at CSU Eastbay was supported in part by Office of Basic Energy Sciences of DOE, and the work at LLNL was carried out under contract number W-7405-Eng-48.

Krishnan Balasubramanian
Lawrence Livermore National Lab

Date submitted: 08 Dec 2008 Electronic form version 1.4