Modeling and Simulation for Separations Processes in Nuclear Fuel Reprocessing

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As part of the US Dept. of Energy's Nuclear Energy Advanced Modeling and Simulation (NEAMS) program, one of the four Integrated Performance and Safety Codes (IPSCs) addresses Safeguards and Separations (SafeSeps) for nuclear fuel cycles. The goal of the SafeSeps IPSC is to assemble a modeling and simulation toolkit that will enable the development and design of commercially viable advanced reprocessing options. I will briefly describe the overall NEAMS program as well as the SafeSeps IPSC element. In the latter half of the talk I will describe: (1) recent quantum chemical studies of the coordination chemistry of lanthanide and actinide cations for separations processes in nuclear fuel reprocessing; (2) the development and deployment of computer-aided molecular software (HostDesigner) for the design of extractant candidates scored with coordination free energies calculated using quantum chemistry techniques.