Materials modeling and simulation of fuels, waste forms and cladding materials

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Abstract:

Grand challenges in the U.S. Department of Energy Fuel Cycle Research and Development (FCR&D) Program include the development of (i) advanced fuels, (ii) cladding materials that can withstand irradiation for extended periods of time, and (iii) optimized waste forms for the waste streams from proposed spent nuclear fuel (SNF) reprocessing strategies.

Computational modeling and simulation at the atomic scale can provide fundamental understanding of the materials/environment interface necessary to develop the predictive capability for fuels, waste forms, and cladding materials performance over a broad range of operational or environmental conditions, thus complementing the indispensable experimental effort.

In this talk I will present recent studies on fuels, waste forms, and cladding materials performed within the framework of density functional theory (DFT). I will discuss about (i) the structural, electronic and thermodynamic properties of actinide nitride fuels, (ii) recent results of candidate Tc waste forms including Tc chalcogenides and lanthanide-technetium pyrochlores as prospective host phases to immobilize 99Tc and fission lanthanides from effluents of reprocessed used nuclear fuels, and (iii) mechanical properties of zirconium alloys and zirconium hydrides.

Bio:

Dr. Eunja Kim is currently an assistant research professor at University of Nevada, Las Vegas (UNLV). She has over 20 years of experience in carrying out fundamental studies of materials that are scientifically interesting and technologically important, including semiconductors, energy storage materials, nuclear fuels, fission products, nuclear waste forms, and cladding materials. Her specialty is in applying density functional theory and ab initio molecular dynamics simulations to investigate the stability and physicochemical properties of energy/device materials, including structural, electronic, vibrational, magnetic, and thermo-mechanical properties. To date, she has authored or co-authored over 110 referred research papers, 9 journal covers, and several Editor's selected highlights in high impact peer-review journals.