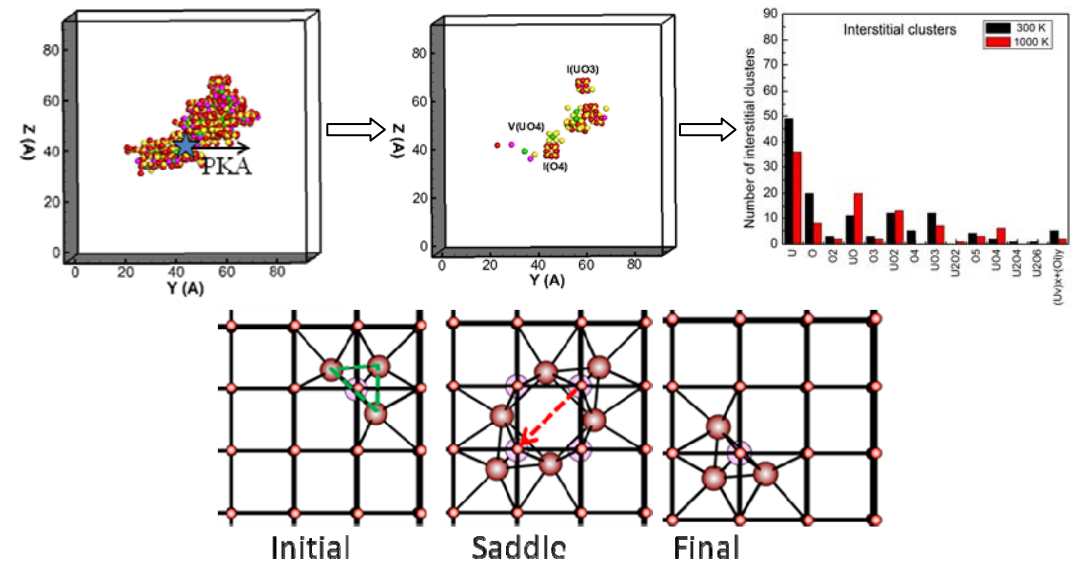
Highlight: Atomistic Simulations of Defect Production and Defect Cluster Diffusion in UO_2



Atomistic studies of defect energetics and kinetics that are related to microstructural evolution of UO_2 under irradiation environment are being performed at Idaho National Laboratory (INL). Dr. **Xianming "David" Bai** (Staff Scientist) at INL uses molecular dynamics (MD) and temperature accelerated dynamics (TAD) to investigate defect production, migration of defect clusters at long timescales, and interaction of point defects with extended defects. Dr. **Jianguo Yu** (Staff Scientist) at INL performs density functional theory (DFT) calculations to investigate defect energetics, kinetics, and stoichiometries near free surfaces in UO_2. Graduate student **Sarah Khalil** at the University of Wisconsin – Madison uses MD and cluster dynamics to study defect clustering through kinetic evolution in UO_2. Undergraduate summer intern **Stephen Taller** at Purdue University conducts MD and molecular statics calculations to investigate the stability of a wide range of defect clusters in UO_2.

Above panel (upper): MD simulations of cascade-induced defect production in UO_2. An algorithm is developed to identify the compositions of these defect clusters. Some special clusters such as cuboctahedral clusters are found to be created directly in cascades. Statistics of the population of point defects and defects clusters are obtained from many simulations.

Above panel (lower): TAD studies of the migration mechanism of a two-oxygen interstitial cluster. The stable di-interstitial cluster consists of an interstitial triangle and a vacancy. At the saddle, a symmetric triangle structure forms. After the migration, the cluster migrates along a <110> direction. The migration barrier of the di-interstitial cluster is found to be much smaller than a single interstitial. Defect clusters of different sizes and types are also investigated. The formation paths of cuboctahedral clusters are then investigated based on the cluster diffusion.

These results can provide inputs for mesocale modeling of microstructural evolution in UO_2 performed at Purdue University within this EFRC program. These works have been presented at the 2011 MRS Fall Meeting in Boston, MA and TMS 2012 meeting in Orlando, FL. Manuscripts are being prepared for the Journal of Nuclear Materials and Physical Review B.