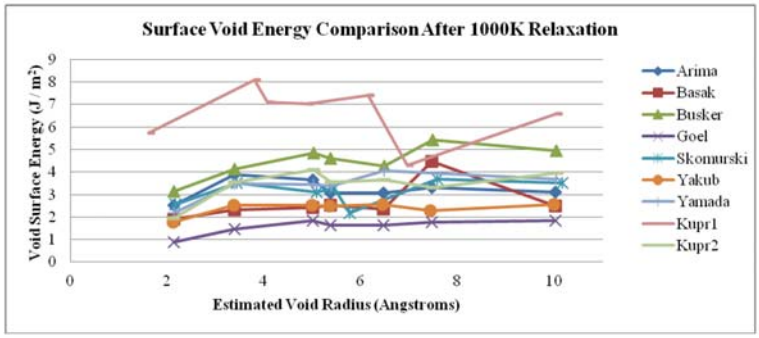
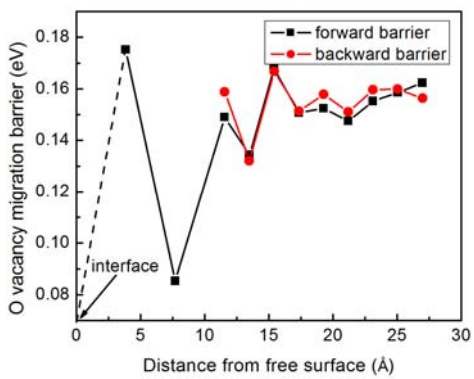
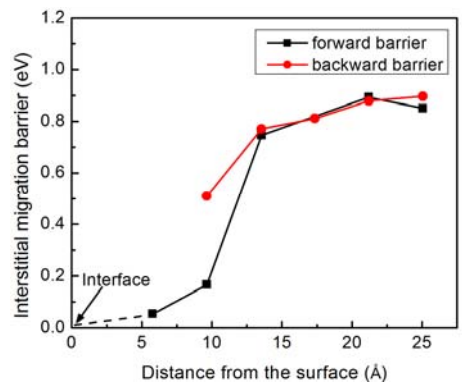
Highlight: Atomistic Investigation of Void Surface Energy Predicted by Different Potentials and Defect Migration towards a Free Surface in UO_2







EFRC researcher **Xianming "David" Bai** (Staff Scientist) at INL and undergraduate summer intern **Stephen Taller** at Purdue University have used atomistic calculations to investigate the defect energetics and kinetics of void surfaces and free surfaces in UO_2. These studies may help us address the EFRC science question "how do voids form and grow in irradiated UO_2 and what is the effect of free surfaces on defect migration?"

(Top panel): The surface energy is a crucial parameter for void nucleation and growth. Stephen Taller and David Bai used molecular dynamics and molecular statics to investigate the void surface energy as a function of void radius predicted by nine empirical potentials. Overall, the void surface energy approaches to a plateau as void radius increases for each potential. However, different potentials predict significantly different surface energies; Most of them are much higher than the experimental value of 1.4 J/m^2, suggesting that choosing an appropriate potential for studying void properties may be important. **(Bottom panel - left)**: David Bai used temperature accelerated dynamics (TAD) to investigate oxygen vacancy migration barriers near a (110) free surface. Since each atomic layer parallel to the (110) surface has a perfect stoichiometry, there is no charge-compensation problem. Both the forward and backward migration barriers are investigated. The vacancy eventually diffuses to the free surface but the migration barrier first decreases then increases to a maximum value before it reaches the surface. This result suggests that the (110) surface may induce an extra barrier for vacancy migration. **(Bottom panel - right)**: Similarly, the oxygen interstitial migration barriers near the (110) surface are also investigated. The barrier decreases monotonically as it approaches to the free surface, suggesting that the free surface accelerates the oxygen interstitial migration. These defect properties will be used as inputs for phase field modeling conducted at Prof. Anter El-Azab's group at Purdue University.