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Migration of rhenium and osmium in tungsten

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We report a series of *ab initio* studies based upon density functional theory for the behavior of rhenium and osmium atoms in body-centered-cubic tungsten crystal. Contrary to the fast one-dimensional migration of self-interstitial atoms, interstitials of these solute elements in tungsten have three-dimensional motion because they form a mixed dumbbell having a low rotation energy barrier. The migration of these solute elements strongly influences the effects of radiation upon the materials, and our results suggest that the low rotation energy barrier leading to three-dimensional migration is a property that is key to the explanation of the radiation effects experimentally observed in tungsten-rhenium and tungsten-osmium alloys.