Stability and migration mechanisms of volatile elements in uranium carbide

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The scope of this study is to shed light on the behavior volatile impurities in uranium carbide, as a first step in the study of the potential Gen IV nuclear fuel (U,Pu)C. The study of point defects and volatile impurities is central in order to get some comprehension in the behavior of the materials under irradiation. Using an *ab initio* method, we calculate and compare the formation energies of the various types of point defects that can be found in UC. Then the behavior of the volatile fission products Kr, Xe and I, as well as O which could be incorporated by oxidation, in UC is studied. The most favorable incorporation traps (vacancies or vacancy clusters) for these elements in the lattice are determined, and the incorporation and migration energies are compared.

All calculations are done using the *ab initio* PAW method (Projector Augmented Waves) based on the DFT as implemented in the VASP code. Exchange-correlation interactions are taken into account within the GGA approximation, and some comparisons are made with the GGA+U approximation.