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New insight into the thermodynamic and atom transport properties of (U,Pu)O_2 nuclear fuel from atomic scale calculations

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The uranium-plutonium mixed oxide (U,Pu)O_2 is currently used as nuclear fuel in pressurized water reactors with a Pu content around 10 wt.%, and is the reference fuel for several Generation IV reactors with a Pu content between 25 and 40 wt.%. A more precise knowledge of the properties of (U,Pu)O_2 and its behaviour under irradiation is needed to refine the models used in the fuel performance codes simulating the behaviour of fuels at the macroscopic scale. A basic research approach coupling detailed characterizations and multiscale modelling starting at the atomic scale can bring significant insight into key phenomena involved in the evolution of nuclear fuels during their reactor life.
We will show the results obtained using state-of-the art electronic structure calculations, including ab initio molecular dynamics simulation, and empirical potential methods on thermodynamic and atomic transport properties of (U,Pu)O_2. In particular, the thermal expansion, mixing enthalpy and specific heat of (U,Pu)O_2 as a function of Pu content will be discussed in view of the available experimental data. The defect properties of (U,Pu)O_2 with 25% Pu as a function of the oxygen-potential will also be presented.

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