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Ab initio calculation of oxygen self-diffusion coefficient in uranium dioxide UO_2 BORIS DORADO, CEA, DAM, DIF - Bruyeres-le-Chatel, France, PHILIPPE GARCIA, CEA, DEN, DEC - Cadarache, France, MARC TORRENT, CEA, DAM, DIF - Bruyeres-le-Chatel, France — Uranium dioxide UO_2 is the most widely used nuclear fuel worldwide and its atomic transport properties are relevant to practically all engineering aspects of the material. Although transport properties have already been studied in UO_2 by means of first-principles calculations, the ab initio determination of self-diffusion coefficients has up to now remained unreachable because the relevant computational tools were neither available or adapted. The present work reports our results related to the ab initio calculation of the oxygen self-diffusion coefficient in UO_2. We first determine the Gibbs free energies of formation of oxygen charged defects by calculating both the electronic and vibrational (hence entropic) contributions. Then, we use the transition state theory in order to compute the effective jump frequency of the defects, which in turn provides us with the value of the pre-exponential factor. The results are compared to self-diffusion data obtained experimentally with a careful monitoring of the relevant thermodynamic conditions (oxygen partial pressure, temperature, impurity content).

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