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Characterization of point defects in UO2 by positron annihilation spectroscopy: a first-principles study MARC TORRENT, GERALD JOMARD, Commissariat a l Energie Atomique et Aux Energies Alternatives, Paris, France — abstract- Positron Annihilation Spectroscopy is a powerful experimental tool for probing defects in crystalline materials. The correct identification of defects with PAS requires the knowledge of accurate positron lifetimes for the various kinds of defects. That can be provided by numerical calculations in the framework of the Two-Component Density-Functional Theory. This method accurately treat on the same footing, the electrons and positron densities as well as the atomic structure. We have implemented this formalism within the Projector Augmented-Wave method in the ABINIT code, optimizing the electrons and positron densities self-consistently and calculating positron-induced forces accurately. That allows to properly determining the relaxed geometries of defects that trapped positron. We have applied the TC-DFT to various point defects in UO2. The use of the PAW method allows considering large super cells to simulate point defects, we have typically used cells that contain 32 UO2 unit formulas. We use the LDA+U framework in order to treat strong electronic correlations. This work is a first attempt to help for the interpretation of PAS experiments on UO2 but it seems really promising.-

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