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Ab initio study of the plutonium dioxide surfaces: role of electronic correlations GERALD JOMARD, FRANCOIS BOTTIN, Commissariat a l'Energie Atomique — This *ab initio* study is performed in the framework of density functional theory (DFT) using the projector augmented wave method. Introducing the on-site Coulomb repulsion term U in the calculations, we found equilibrium properties of both PuO_2 and Pu_2O_3 in good agreement with experiments. At odds with conventional DFT calculations, these two compounds are no more metallic and recover their insulating behavior with an antiferromagnetic order. As concerns the surface properties of the plutonium dioxide PuO_2, we perform an extensive study of eleven (1×1) (110), (100) and (111) terminations then compare their thermodynamic stability by computing their surface Grand potential. Whereas conventional DFT calculations predict that a few uncompensated polar terminations can be stable, in the stability domain of the PuO_2 compound, the inclusion of the electronic correlations modify significantly these conclusions. We discuss this result by connecting the surface electronic structure to the polar or non-polar character of the termination.

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