GGA+U study of uranium mononitride: A comparison of the U-ramping and occupation matrix schemes and incorporation energies of fission products

Abstract:
Uranium mononitride is studied in the DFT+U framework. Its ground state is investigated and a study of the incorporation of diverse fission products in the matrix is conducted. Due to the existence of metastable states, a procedure has to be implemented to ensure that the ground state is reached. The schemes known as U-ramping and occupation matrix control (OMC) are used and compared. Their results are similar up to a certain amount of introduced correlation, at which point the OMC scheme starts to and a lower total energy. Based on this fact and on the more modest computational effort needed using this method, the OMC is chosen for the second part of this study. Before that, the influence of the magnetic ordering is studied using the U-ramping method, showing that antiferromagnetic (AFM) order is the most stable one when the U parameter is larger than 1.75 eV. The effect on the density of states is investigated and elastic constants are provided for comparison with other methods and experiments. The incorporation energies of fission products in different defect configurations are calculated and these energies are corrected to take into account the limited size of the supercell.

URI:

Authors:
CLAISSE Antoine
KLIPFEL Marco
LINDBOM Niclas
FREYSS Michel
OLSSON Per

Publication Year:
2016

Science Areas:
Nuclear safety and security

Keywords:
actinide