Παρουσίαση διπλωματικής εργασίας

Παρασκευή 28/1/2022 και ώρα 12:00

https://authgr.zoom.us/j/95284659174

Title : The influence of antimony (Sb) atoms as a dopant in ZnO using atomistic modeling and DFT based simulations

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Abstract : Zinc oxide is one of the most popular materials in science and technology. It is widely used in various optical, electrical, magnetic and energy devices as its application areas basically encompass all areas of engineering. Although the doping of ZnO is still under debate, multiple dopants have been studied and their related applications as functional materials are numerous. ZnO dopants will vary depending on the application target. In this thesis, the influence of antimony (Sb) atoms as a dopant in ZnO is studied. To further study the structure of crystal defects, density function theory (DFT) is very valuable. The wurtzite structure of ZnO as well as the various structures of antimony oxides are studied using the VASP code with projector augmented-wave (PAW) potentials along with the Perdew-Burke-Ernzerh derivation of the generalized gradient approximation (GGA-PBE) and the GGA+U approach. Various atomistic configurations are investigated in order to establish the energetically favorable one as well as the corresponding electronic properties.

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