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Experimental and ab initio study of Ta-doped ZnO semiconductor

In the last years, ab initio calculations performed in the framework of the Density Functional Theory (DFT) have been successfully applied to the study of doped oxide semiconductors. The Full-Potential Augmented Plane Wave plus local orbitals (FP-APW+lo) method enables to determine the Electric-Field-Gradient tensor (EFG) at impurity sites localized in cation sites of the host structure with very good precision. From an ab initio - experimental study, the electronic structure and structural relaxations produced by the inclusion of the Perturbed Angular Correlation (PAC) tracers in the host system can be determined [1,2,3] . In this work, we present PAC results in polycrystalline ZnO semiconductor implanted with (181Hf→)181Ta probes. The FP-APW+lo calculations in Ta-doped ZnO were carried out using the supercell method and varying self-consistently the charge state of the impurity. Ta is a triple donor impurity with respect to Zn2+ in ZnO and thus it can loose 1, 2 o 3 donor electrons under certain circumstances. The comparison between the experimental EFG results and our ab initio predictions suggests that the Ta impurity may be in a completely ionized charge state, i.e., with the 3 donor electrons removed from the impurity.

Are you a student, a delegate from developing countries or a participant with physical needs and would like to apply for a sponsored accomodation. Please answer with yes or no.

YES

Please specify whether you would prefer an oral or poster contribution.

poster contribution

Summary

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