

Dynamic Hyperfine Interactions in ($^{111}\text{In} \rightarrow$) ^{111}Cd -doped SnO_2 and SnO Semiconductors: *Ab Initio* Approach to the Electron-Capture After-Effects Phenomenon

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In the PAC literature, the so-called “after-effects” phenomenon refers to the electronic relaxations processes of a probe-atom following the electron-capture (EC) nuclear-decay of its radioactive parent. This effect has been observed in PAC experiments on semiconducting and insulating oxides doped with $^{111}\text{In}(\rightarrow^{111}\text{Cd})$, through the existence of *dynamic* hyperfine interactions (i.e., with time-dependent anisotropies), dependent and reversible with measuring temperature. We present here results of PAC experiments in ($^{111}\text{In} \rightarrow$) ^{111}Cd -doped SnO_2 and SnO that have been successfully analyzed with a time-dependent *on-off* model for the perturbation factor. These results showed combined *dynamic* plus *static* hyperfine interactions whose electric-field gradients (EFG) were associated to different stable electronic configurations close to the ^{111}Cd nucleus. The *dynamic* regime is originated in fast fluctuations between these different electronic configurations. Density functional theory-based electronic-structure calculations of Cd-doped SnO_2 and SnO were performed as a function of the charge state of the impurity. In SnO_2 , the impurity introduces a double acceptor level in the top of the valence band together with isotropic outward relaxations of the nearest oxygen neighbors. The variation of the calculated EFG tensor as a function of the charge state of the Cd impurity level shows an interesting behavior that explains the experimental results, giving strong support from first principles to the electron-capture after-effects proposed scenario. A similar *ab initio* analysis in Cd-doped SnO , in which Cd is nominally an isovalent impurity, also gave account successfully of the experimental results.

The EC decay of ^{111}In to ^{111}Cd and the electric nature of the host are shown to contribute to the existence of these types of time-dependent hyperfine interactions, showing that the acceptor character of the impurity seems not to be a necessary condition to produce *after effects* at least in Sn oxides.