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Ambipolar Property of Isolated Hydrogen in Oxide Materials Revealed by Muon

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The study on the electronic state of muon as pseudo-hydrogen (represented by the elemental symbol Mu) by muon spin rotation has long been appreciated as one of the few methods to experimentally access the electronic state of dilute hydrogen (H) in semiconductors and dielectrics. Meanwhile, theoretical predictions on the electronic state of H in these materials by first-principles calculations using density functional theory (DFT) do not always agree with the observed states of Mu. In order to address this long-standing issue, we have re-examined the vast results of previous Mu studies in insulating/semiconducting oxides with special attention to the non-equilibrium character and the ambipolarity of Mu. As a result, we established a semi-quantitative model that enables systematic understanding of the electronic states of Mu in most oxides.
First of all, Mu often occurs simultaneously in a neutral (Mu^0) and a diamagnetic state (Mu^+ or Mu^-) in wide-gap oxides, which is not explained by DFT calculations that predict only diamagnetic states with the polarity determined by the equilibrium charge-transition level ($E^{+/-}$). Our model considers that μ^+ interacts with self-induced excitons upon implantation to form relaxed-excited states corresponding to a donor-like (Mu_D) and/or an acceptor-like (Mu_A) states. Moreover, these states are presumed to accompany the electronic level ($E^{+/0}$ or $E^{-/0}$) predicted by the DFT calculations for H. By considering that the stability of these two states including their valence is determined by i) the relative position of $E^{\pm/0}$ in the energy band structure of the host and ii) a potential barrier associated with the transition between Mu_D and Mu_A, we find that the known experimental results can be explained systematically in accordance with $E^{\pm/0}$. The model also provides new insights into the polaron-like nature of the electronic states associated with shallow donor Mu complexes and the fast diffusion of Mu_A^0.

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