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Ab initio calculations of positron lifetimes and the comparison with lifetime measurements in photochromic rear-earth oxihydrides

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Rare-earth oxihydrides show a reversible photochromic effect, whereas the details of the underlying mechanism are not yet fully understood. A major influence on properties such as band gap, electrical conductivity, or light absorption is achieved by modifying the chemical composition, i.e. the O^{2-} and H content of the material. Recently published results of PALS measurements performed with the Pulsed Low-Energy Positron System (PLEPS) at the research reactor FRM II on magnetron sputtered Yttrium-based thin films report the occurrence of different positron defect lifetimes in the materials. Very often, such results are difficult to interpret because, especially in complex materials, different defect types may lead to similar positron lifetimes. Therefore, ab initio calculations, based on ABINIT were performed for further interpretation. ABINIT is an open-source software suite that uses density functional theory (DFT) using a plane wave basis set and pseudopotentials. With an additional package, self-consistent field calculations can be performed to determine positron lifetimes based on two-component density functional theory (TCDFT) using the projector augmented-wave (PAW) method. For our calculations, we used the local density approximation (LDA) and the generalized gradient approximation (GGA). The calculations and our measured data show a high degree of agreement. Furthermore, the DFT results help us to interpret the results.

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