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Supporting information for article:

Influence of core-hole effect on optical properties of Magnesium Oxide (MgO) near Mg L edge region

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S1. Origin of the formation of core-exciton states

When a photon having an energy equivalent to the Mg L edge energy gets impinged on MgO, formation of core-hole occurs at Mg L shell as a result of knocking out of an electron. After the formation of the core hole, it may be screened by the surrounding electron cloud present in the system leading to the formation of bound exciton states. The main principle behind the formation of these states can be attributed to the Coulomb interaction between the excited electron and the core hole formed. Since these bound exciton states are localized deep within the atomic cores and are incapable of hopping from one atomic site to another, these can be named as core-exciton states. The electron associated with a core exciton faces an excess strong potential of the core-hole as a result of which an observable change in the electronic structure near the vicinity of the absorption edge can be noticed. However, the strength of the core-exciton effects may vary from system to system (e.g; semiconductor, insulators). The degree of the effect primarily depends on the response of the remaining electrons in the solid that attempt to screen the core hole from the high-energy unoccupied states. Thus, in case of insulators the core-hole effect plays a key role in the modifications of the electronic structures near the vicinity of the absorption edges as compared to metals and semiconductors. There are ample of literatures showing the core-exciton features in the absorption spectrum, especially near the edge region. The theory of the absorption spectrum is based on the famous principle of quantum mechanics- the Fermi Golden rule, where two factors such as, site and symmetry projected density of states and the transition matrix elements plays the major role. However, the origin of the features corresponding to the core-hole effect can't be completely interpreted from these two terms. In order to understand this, we present a schematic understanding of the core-hole or equivalently core-excitonic effect in our case.

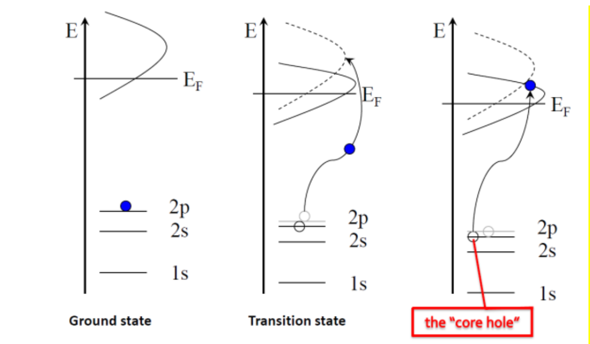

Figure S1 Schematic representation of the formation of a core-exciton state as a consequence of core-hole effect.

The figure at the left shows the ground state (or initial state) - with the electron of the 2p state being excited by the x-ray photon. The middle figure shows that an electron making a transition to the unoccupied valence states are pulled down in energy due to the presence of the hole in the 2p state. The curve on the right is the spectrum in the final state with a hole in the 2p and a photoelectron in the valence band shifted down in energy due to the attractive core hole. This fact is evident in the Figure 5, where we can clearly observe that the calculated absorption spectrum considering core-hole is slightly shifted in energy as compared to the spectrum calculated in absence of core-hole. We have not shown explicitly the above in the density of states separately (DOS of MgO in presence & absence of core-hole) because each peak in the DOS becomes overlap of the dashed and solid curves of the right hand figure of the above schematic.

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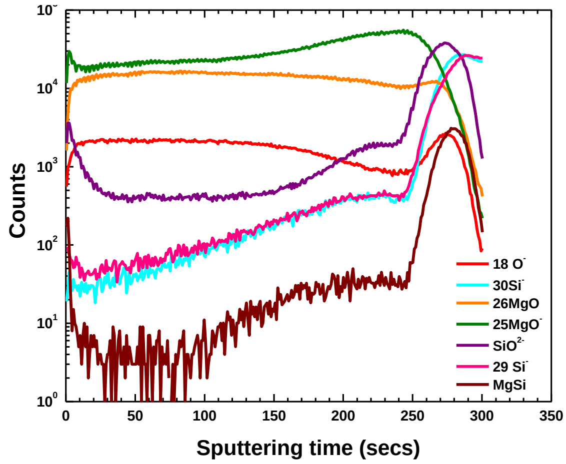

Figure S2 Secondary ion mass (SIMS) spectra of magnesium oxide (MgO) thin film.

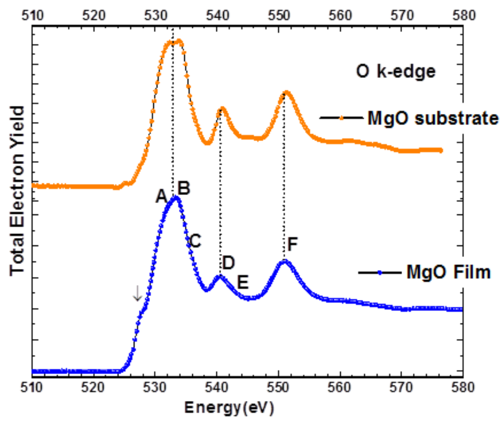

Figure S3 X-ray absorption spectra of 500 Å thick MgO thin film and that of a MgO substrate measured in total electron yield (TEY) mode near the O-K absorption edge region.