

Supplementary Information.

The DOS and PEDOS for the Cu vacancy (Figure 1), and for the Sr vacancy (Figure 2) are shown below. It is clear from both PEDOS that the hole states are composed of Cu *d* and O *p* states.

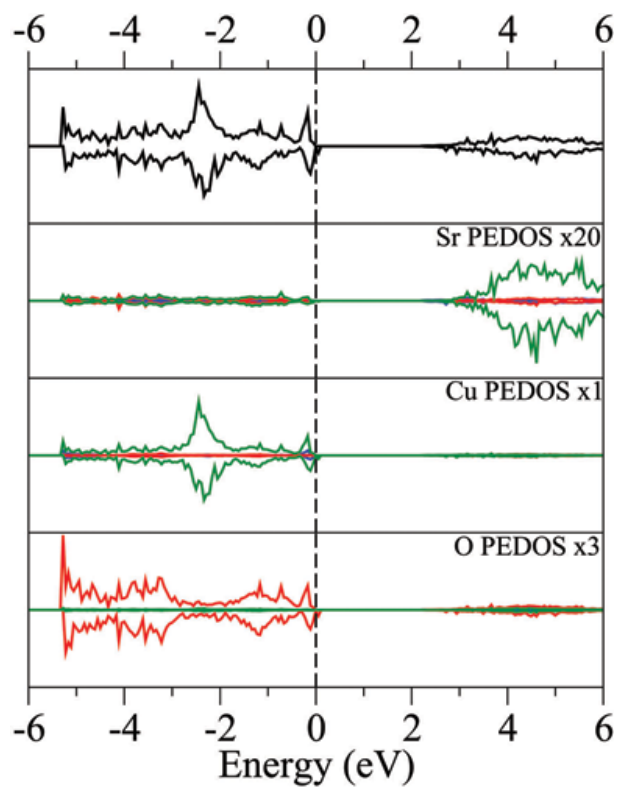


Figure 1: DOS and PEDOS for  $V_{Cu} + h^\bullet$  defect with *s* states in blue, *p* in red and *d* in green. Dashed line indicates highest occupied level.

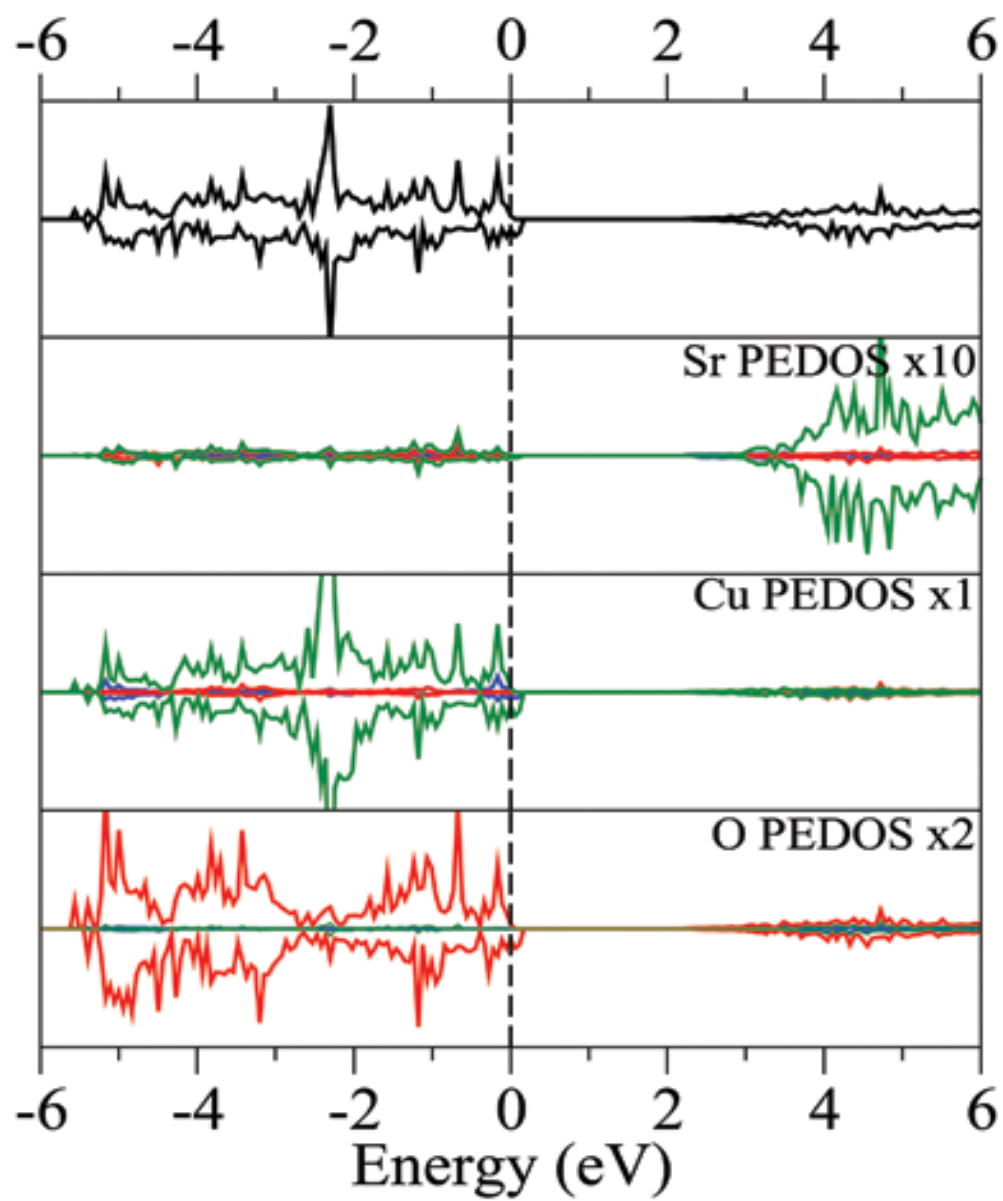


Figure 2: EDOS/PEDOS for  $V_{Sr}^{2+} + 2h^{\bullet}$  with  $s$  states in blue  $p$  states in red and  $d$  states in green. A dashed line indicates highest occupied level.