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## Development of Enduring Interstitial Defects in Mg Doped CuO Thin Films

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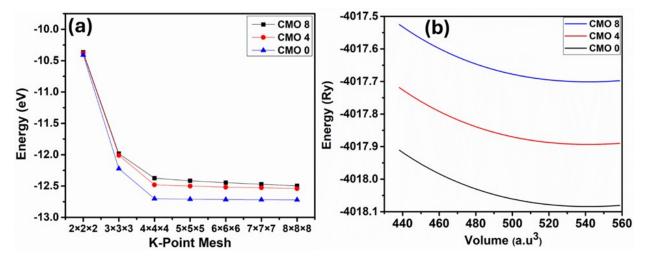


Fig S1: (a) K-point and (b) volume optimization.

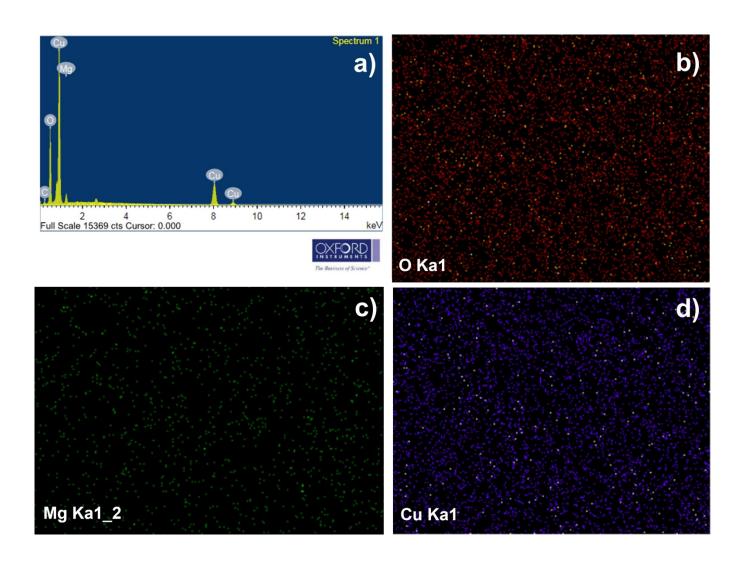


Fig S2: Representative a) EDAX spectrum, elemental mapping of b) O, c) Mg, d) Cu of CMO 8 sample

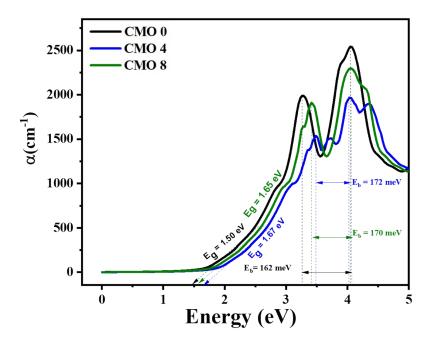


Fig S3: Simulated optical spectra of (a) CMO  $\theta$  (b) CMO 4 and (c) CMO  $\theta$ 

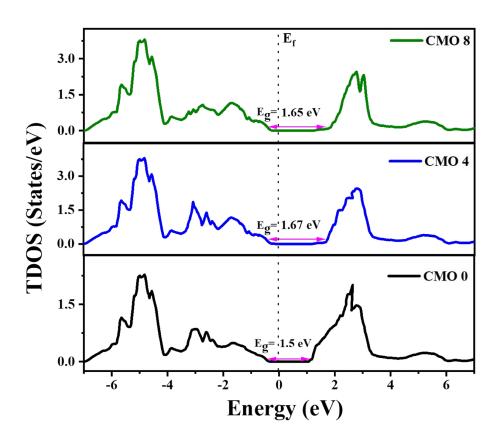


Fig S4: Total density of states of (a) CMO  $\theta$  (b) CMO 4 and (c) CMO 8