

Supporting Information

High Structural Stability, Reduced Lattice-Thermal Conductivity, and Elevated Energy Harvesting Efficiency in a $\text{Lu}_2\text{CoCrO}_6$

Samia Shahzadi¹, A. Elfasakhany², and S. Nazir^{1*}

¹*Department of Physics, University of Sargodha, 40100 Sargodha, Pakistan and*

²*Mechanical Engineering Department, College of Engineering, Taif University, Taif 21944, Saudi Arabia*

* Electronic address: safdar.nazir@uos.edu.pk, Tel: +92-334-971-9060

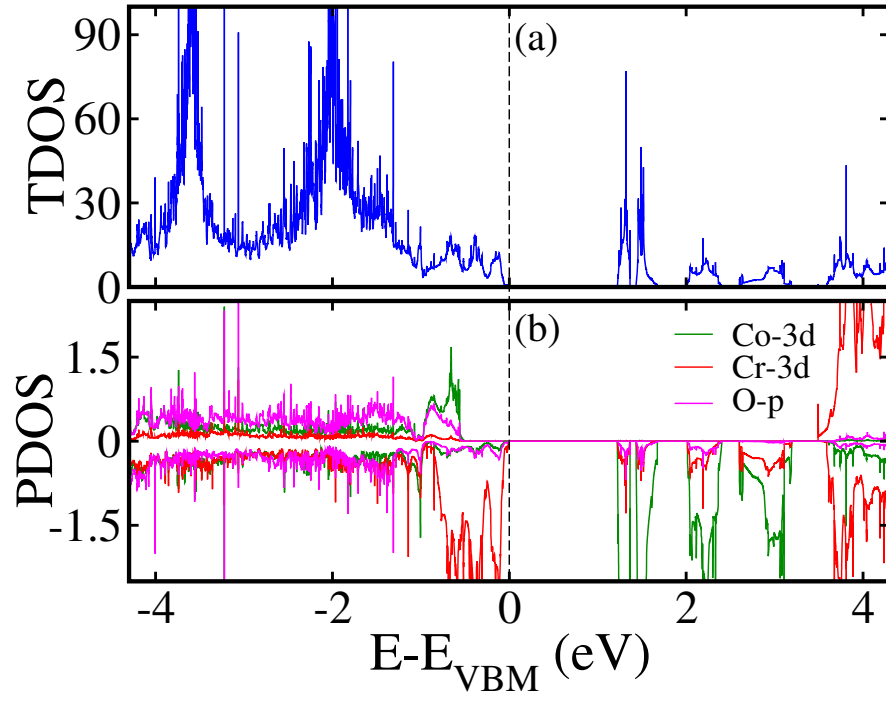


FIG. 1S: (Color line) GGA+ U +SOC calculated (a) total density of states (TDOS) and (b) partial density of states (PDOS), highlighting the role of Co-3d/Cr-3d/O-2p orbitals around the Fermi level for the $\text{Lu}_2\text{CoCrO}_6$ structure.