

# ADVANCED FUNCTIONAL MATERIALS

## Supporting Information

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### Charge-Compensated Compound Defects in Ga-containing Thermoelectric Skutterudites

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This supporting information includes:  
**Figure S1**

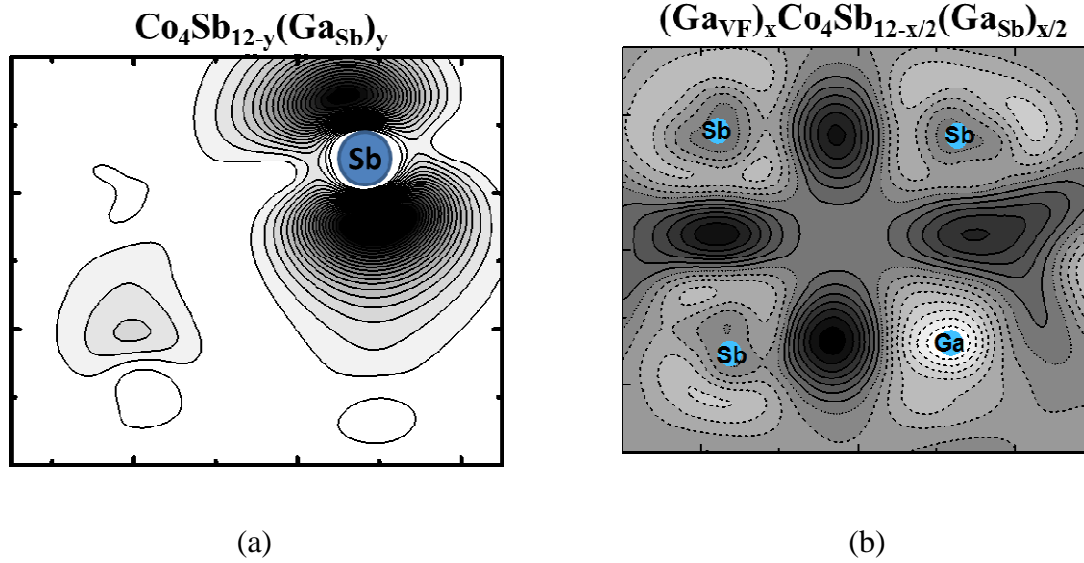


Figure S1 (a) Charge density distribution of the Ga-substitution-induced unoccupied flat and in  $\text{Co}_4\text{Sb}_{12-y}(\text{Ga}_{\text{Sb}})_y$  system shows clearly a localized dangling bond picture. (b) Bonding picture in the charge-compensated system  $(\text{Ga}_{\text{VF}})_x\text{Co}_4\text{Sb}_{12-x/2}(\text{Ga}_{\text{Sb}})_{x/2}$ .