Supporting Information


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 Co$_4$Sb$_{12-y}$Ga$_y$Sb$_{12-y}$ system shows clearly a localized dangling bond picture. (b) Bonding picture in the charge-compensated system (Ga$_{VF}$)$_x$Co$_4$Sb$_{12-x/2}$Ga$_{x/2}$Sb$_{12-x/2}$.