

Supporting information for

## Origin of doping enhanced thermoelectric properties of CrSi<sub>2</sub>

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### Table: - ST1

Formation energies of neutral defects:

Dopants	Formation energy (eV)	Reference Material	Doping %
Al <sub>Si</sub>	0.17	Al bulk	4
P <sub>Si</sub>	0.50	PH <sub>3</sub>	4
V <sub>Cr</sub>	0.47	V bulk	4
Mn <sub>Cr</sub>	0.67	Mn bulk	4
Fe <sub>Cr</sub>	0.17	Fe Bulk	4

### Table: - ST2

DFT lattice parameters for the reference materials:

Reference Material	DFT lattice parameter (Å)	Experimental lattice parameter (Å)
Al	4.15	4.05 <sup>[1]</sup>
PH <sub>3</sub>	6.43	6.31 <sup>[2]</sup>
V	2.97	3.02 <sup>[3]</sup>
Mn	8.85	8.91 <sup>[4]</sup>
Fe	3.48	3.43 <sup>[5]</sup>
Cr	3.65	3.60 <sup>[5]</sup>
Si	5.50	5.43 <sup>[6]</sup>

### Table: - ST3

Defect transition level and corresponding activation temperature:

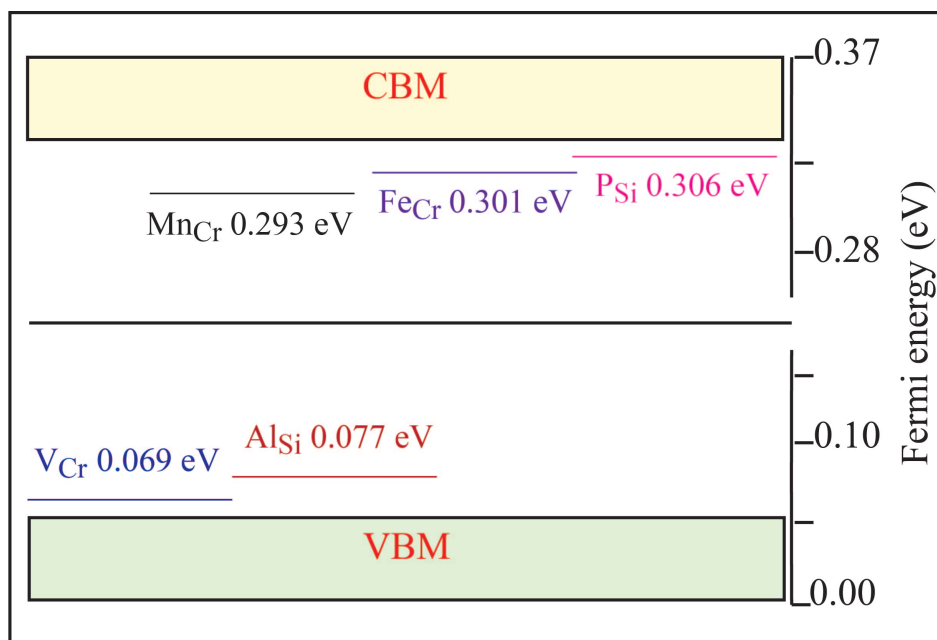
Dopants	Transition level (eV)	Activation temperature (K)	T <sub>m</sub> <sup>*</sup> (K)
Al <sub>Si</sub>	0.077 (From VBM)	900	900
P <sub>Si</sub>	0.064 (From CBM)	750	750
V <sub>Cr</sub>	0.069 (From VBM)	800	800

Mn <sub>Cr</sub>	0.077 (From CBM)	900	900
Fe <sub>Cr</sub>	0.069 (From CBM)	800	800

\*  $T_m$  is the temperature at which thermopower peaks. As shown in the table this temperature is closely related to the temperature which corresponds to position of defect transition level.

### Fig. S1-

The position of defect transition levels across the band gap for different dopants. The dopants and corresponding defect transition levels are denoted on the top of line.



### Details of Rigid Band Model Approximation:

To compare with explicit doping results with RBA, we model same doping level under RBA. As explained the doping levels are used for explicit doping are 4%. A doping level 0.12 (n, p/unit cell) is used for Al, P, Mn and V cases. Since Fe doping donated 2 electrons to sample to match the carrier concentration accurately a doping level of 0.24 (n/unit cell) is used in Fe doped case. Since there are three formula units per cell, our assumed doping levels for these calculations give rise to same carrier concentrations.

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