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Correlation between defect transition levels and thermoelectric operational temperature of doped $CrSi_2$[1] ABHISHEK SINGH, TRIBHUWAN PANDEY, Indian Institute of Science — The performance of a thermoelectric material is quantified by figure of merit ZT. The challenge in achieving high ZT value requires simultaneously high thermopower, high electrical conductivity and low thermal conductivity at optimal carrier concentration. So far doping is the most versatile approach used for modifying thermoelectric properties. Previous studies have shown that doping can significantly improve the thermoelectric performance, however the tuning the operating temperature of a thermoelectric device is a main issue. Using first principles density functional theory, we report for $CrSi_2$, a linear relationship between thermodynamic charge state transition levels of defects and temperature at which thermopower peaks. We show for doped $CrSi_2$ that the peak of thermopower occurs at the temperature T_m, which corresponds to the position of defect transition level. Therefore, by modifying the defect transition level, a thermoelectric material with a given operational temperature can be designed.

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