Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

"Thermodynamics, kinetics and electronic properties of point defects in β-$FeSi_2$"

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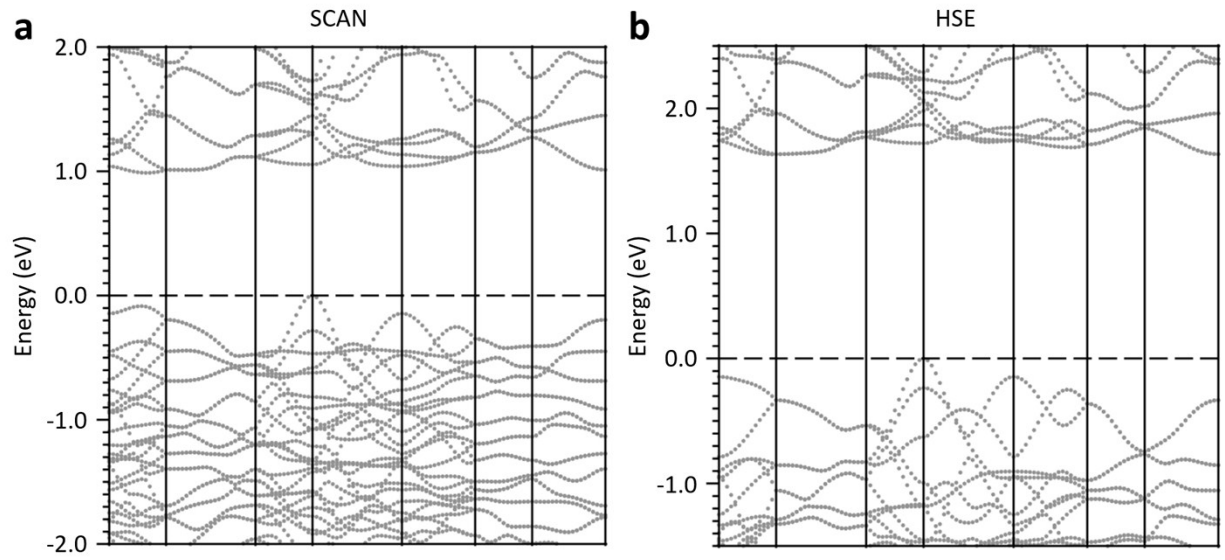

Figure S1. Band structure of β-$FeSi_2$ calculated by SCAN (a) and HSE (b) functional, using structures optimized by the SCAN functional.

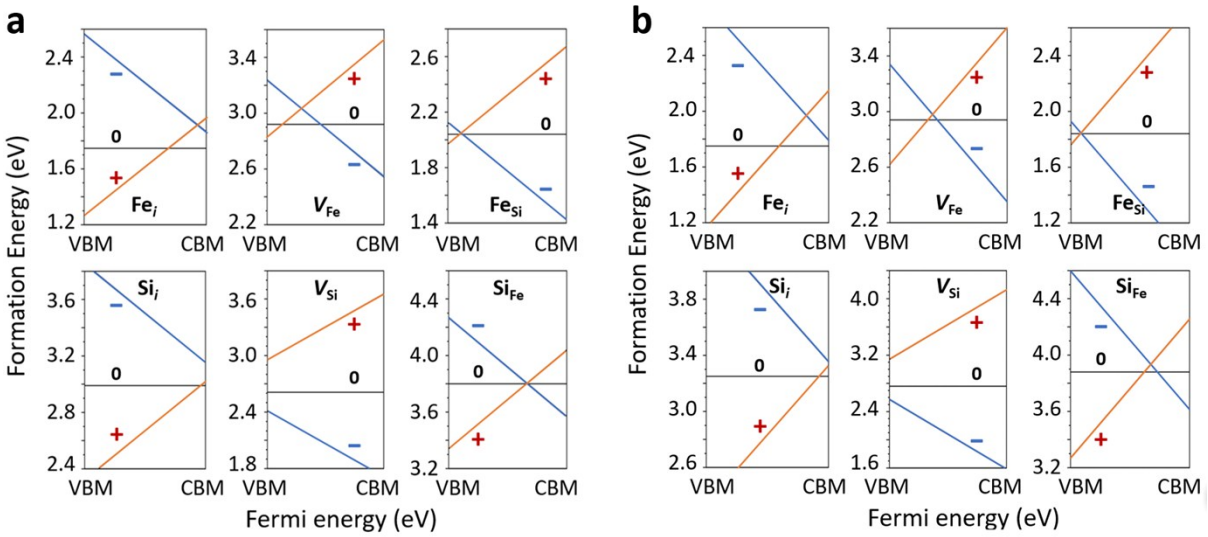

Figure S2. Calculated formation energy of neutral and charged defects in β-$FeSi_2$ as a function of Fermi energy of the system. (a) Results obtained by using PBE functional. (b) Results obtained by using SCAN functional. The results were obtained using a 96-atom supercell.

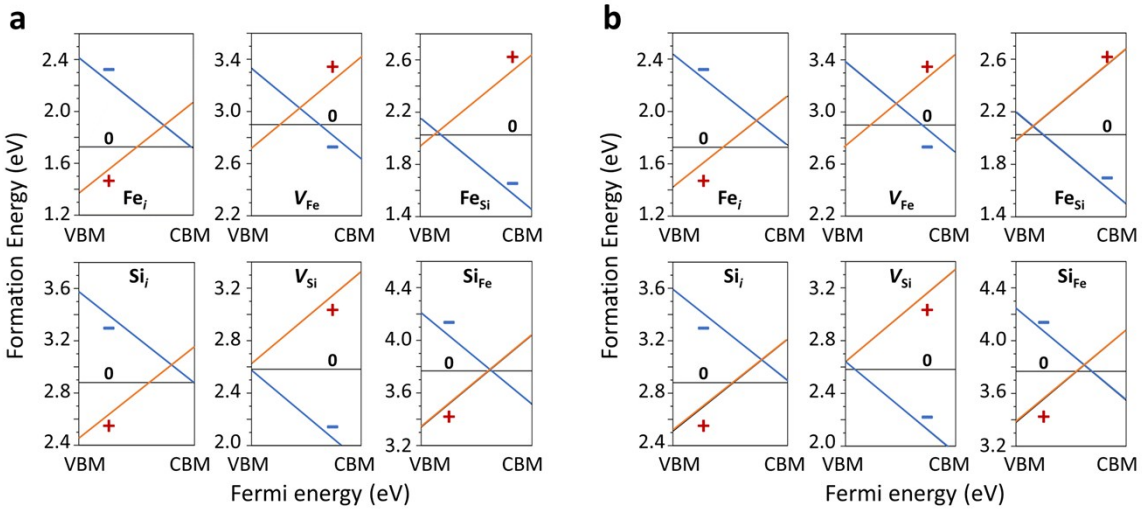

Figure S3. Calculated formation energy of neutral and charged defects in β-$FeSi_2$ as a function of Fermi energy of the system without (a) and with (b) the correction from the sxdefectalign program. The results were obtained using a 768-atom supercell.

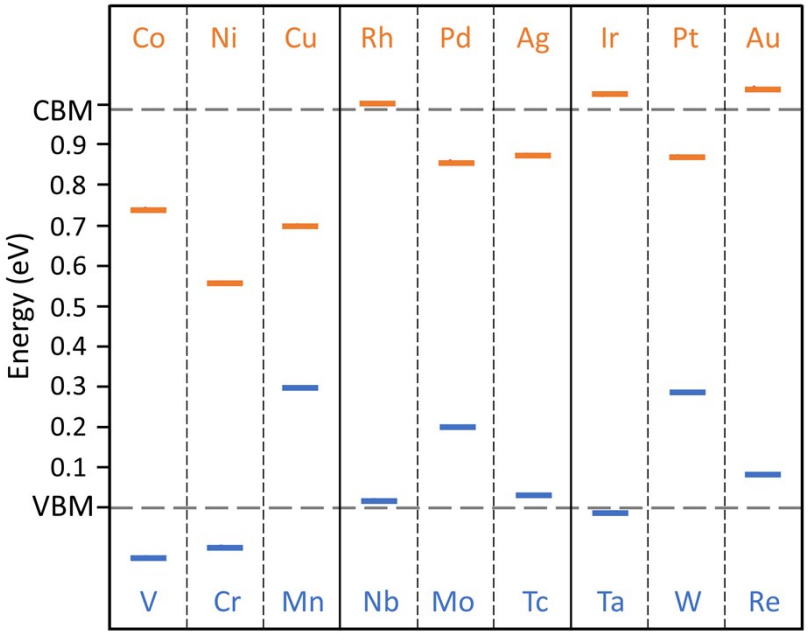

Figure S4. Defect transition levels of Fe-site impurities calculated by using the SCAN functional and a 96-atom supercell. Donor levels are marked by brown color. Acceptor levels are marked by blue color.