Defect calculation of ZnM_2O_4 (M = Rh, Ir) spinel corrected by FERE correction using meta-GGA-SCAN

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[1]$ZnRh_2O_4$ is a material expected to be used as a p-type transparent semiconductor. There are far fewer types of p-type transparent semiconductors than n-type transparent semiconductors, and it has been difficult to form p-n junctions to create a variety of semiconductor functions.

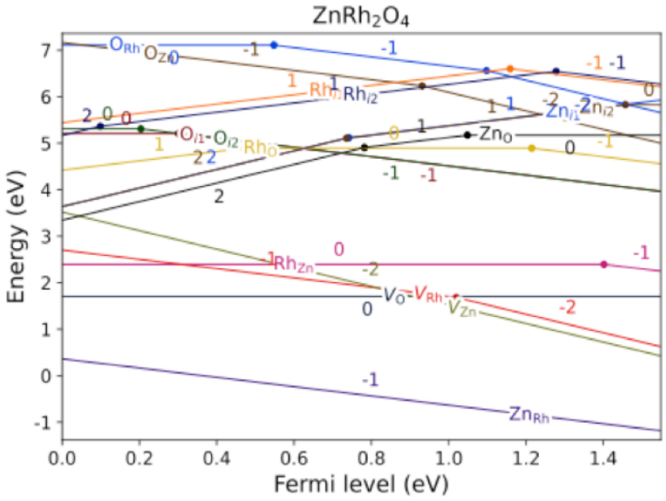

Fig. 1 Calculated formation energy diagram of various defects added to $ZnRh_2O_4$ with FERE correction

Therefore, to confirm whether $ZnRh_2O_4$, which is expected to be a transparent oxide semiconductor that tends to become p-type, is practical, we decided to use SCAN, a relatively new method for defect calculation. Furthermore, to predict the formation energy more accurately, we applied [2]Fitted Elemental-phase Reference Energies (FERE) correction, which corrects the formation energy error between metals and nonmetals that potentially appears in DFT calculations.

Figure 1 is a defect formation energy diagram in an O-rich, Rh-poor environment drawn by [3]pydefect, which supports point defect calculation, with FERE correction applied.

References

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