Supplementary Material (ESI)

Computational Insights into the Structural and Electronic Properties of First-Row Transition Metal-Doped In_2O_3 Systems

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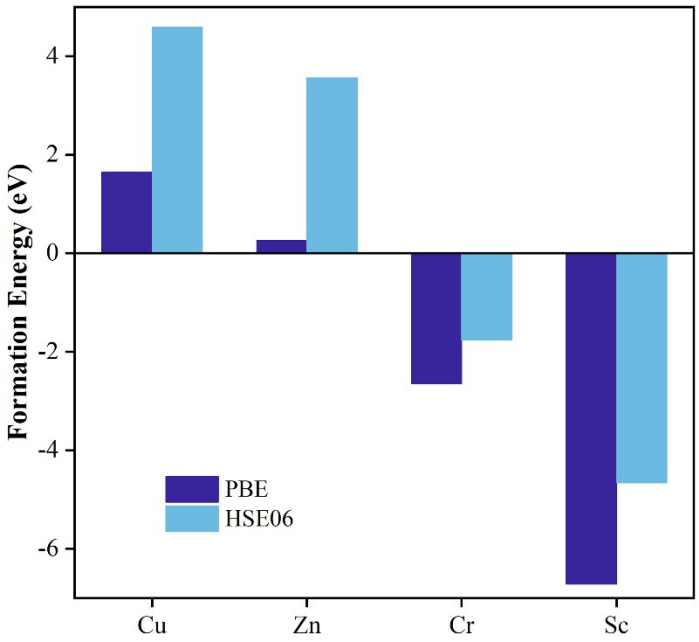

Figure S1. Comparison of formation energy calculated with PBE and HSE06 functionals.

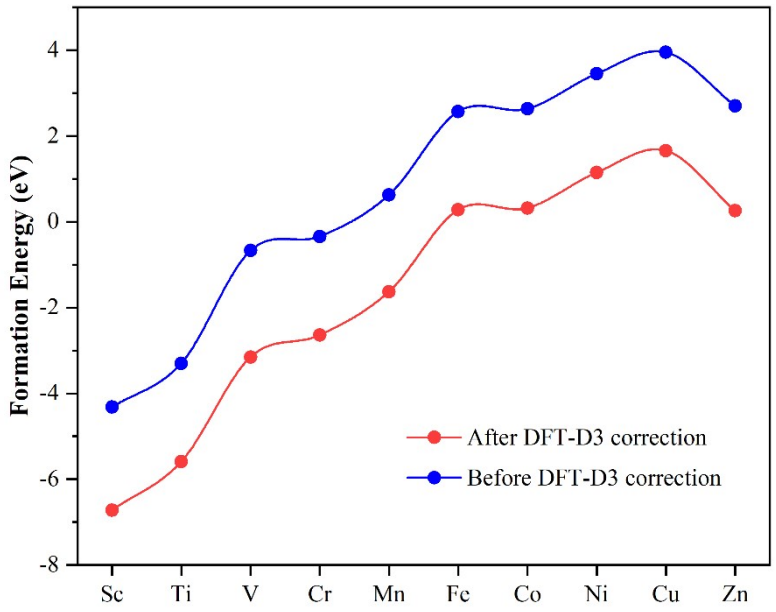

Figure S2. Comparison of formation energies for 3*d* TM-doped In_2O_3 calculated without (top points) and with (bottom points) DFT-D3 dispersion correction.

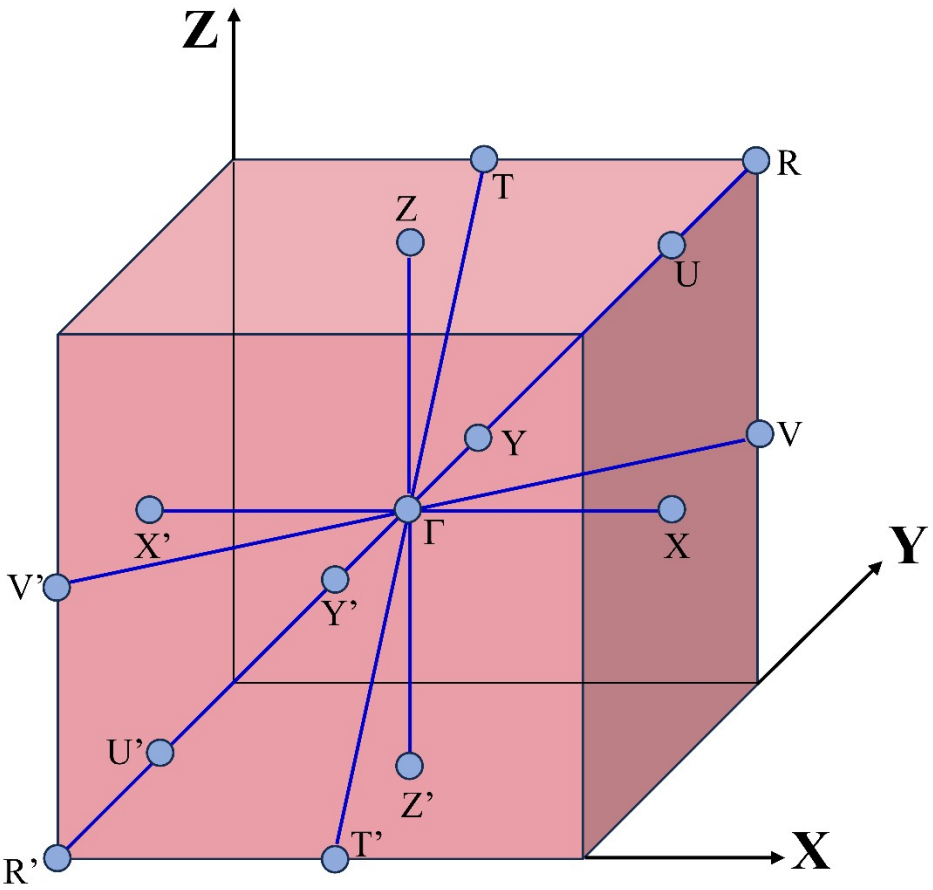

Figure S3. High-symmetry *k*-paths in the reciprocal space of Sc-doped In_2O_3.

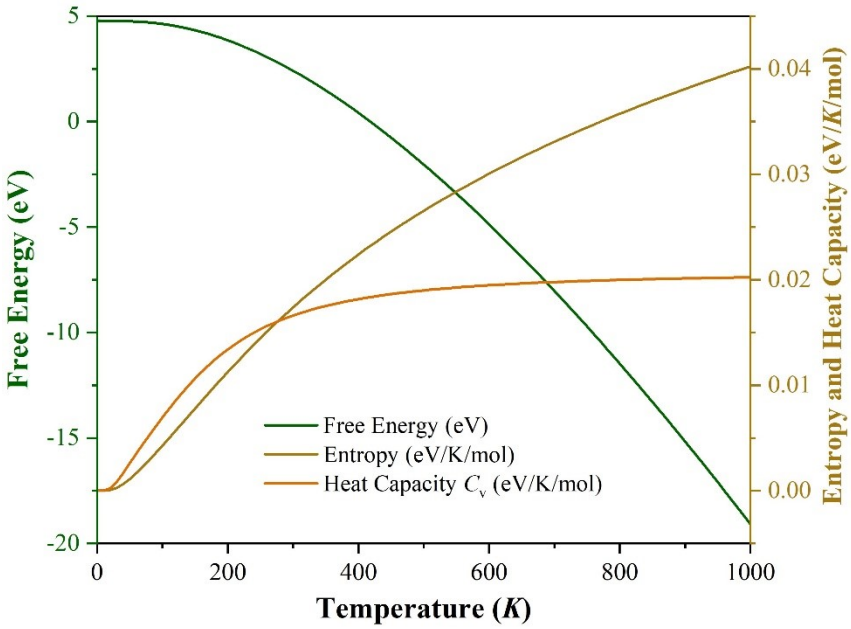

Figure S4. Thermodynamic properties of Sc-doped In_2O_3 as a function of temperature. The green curve is the Helmholtz free energy (left Y-axis), the brown curve is the entropy (right Y-axis), and the orange curve is the heat capacity C_v (right Y-axis).