Supporting materials

Structural stability characteristics and electronic properties of 001 surface with point defects of Zinc Stannate: A first-principle study

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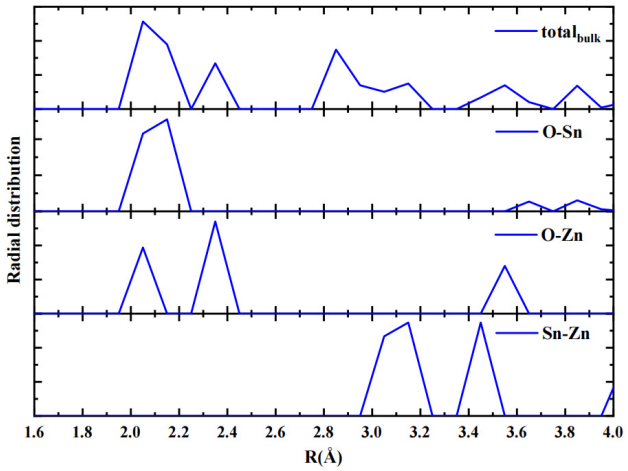

Figure S1. The radial distribution functions of zinc stannate bulk

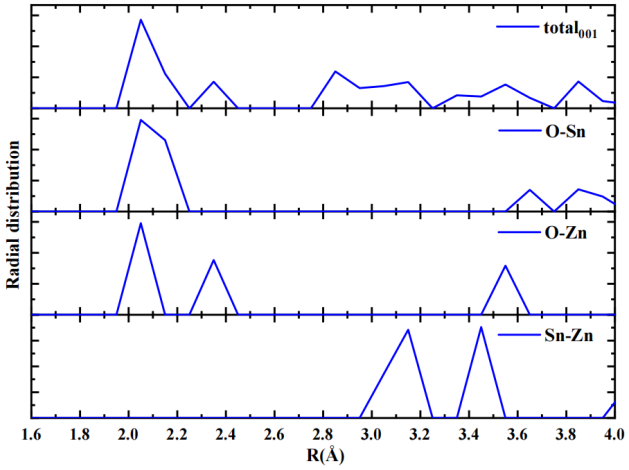

Figure S2. The radial distribution functions of the 001 perfect surface

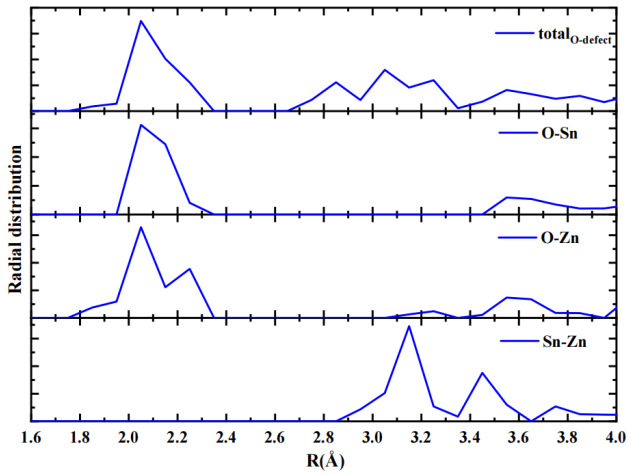

Figure S3. The radial distribution functions of the O defect

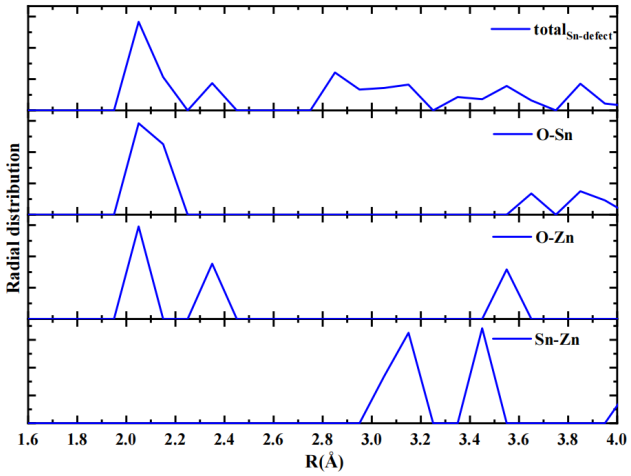

Figure S4. The radial distribution functions of the Sn defect

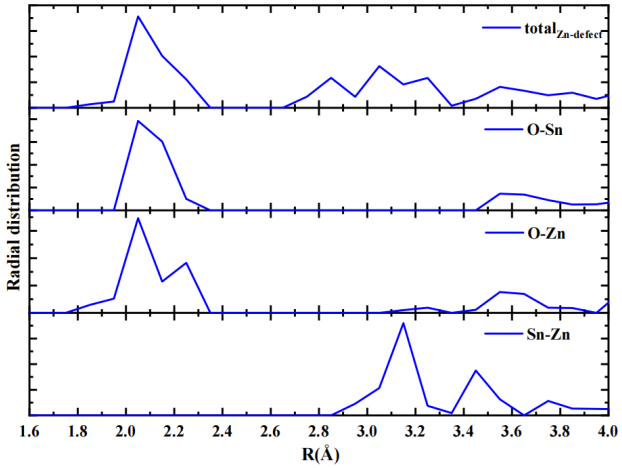

Figure S5. The radial distribution functions of the Zn defect

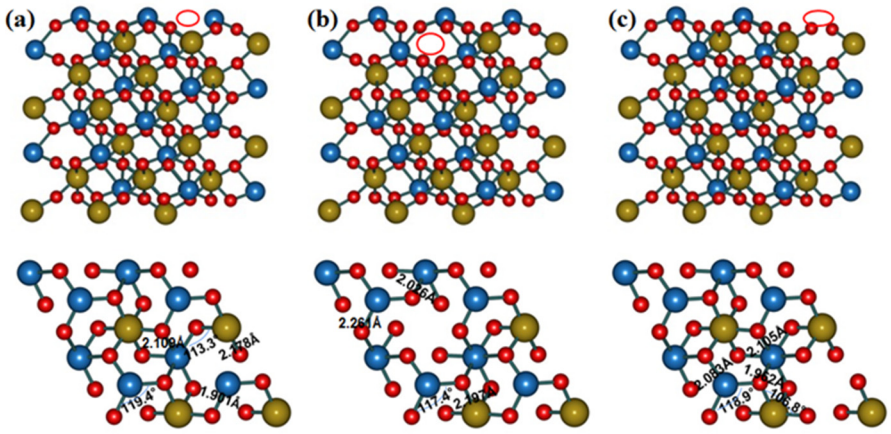

Figure S6. Structures of O defect (a), Sn defect (b), Zn defect (c) on 001 surface of ZS. The defect locations are marked with red circles. Below the three defect models correspond to the top view of defects after structure optimization.

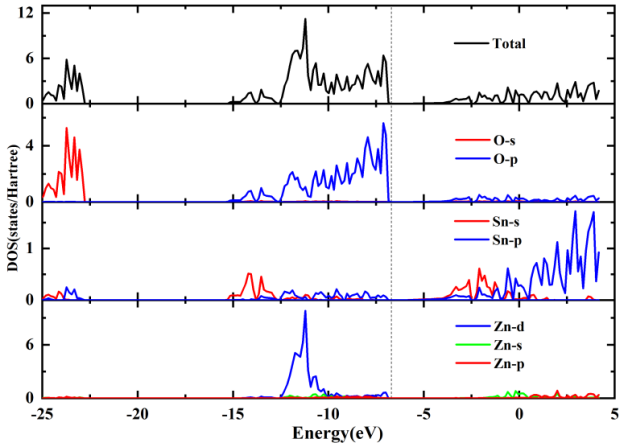

Figure S7. Total and Partial Density of States of $ZnSnO_3$ Bulk