Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplemental Material

Insights on the electronic structure of Tin (II) pyrochlore oxides with $5s^2$ lone pair states as transparent p-type oxide semiconductors

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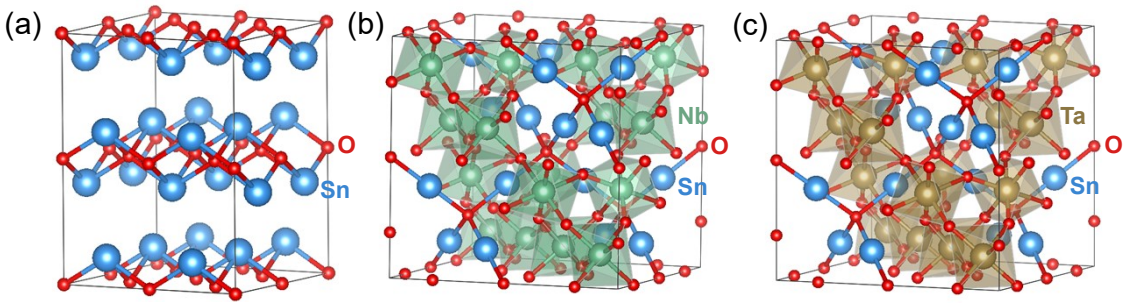

Figure S1. The crystal structure (a) litharge SnO; (b) pyrochlore $Sn_2Nb_2O_7$ and (c) pyrochlore $Sn_2Ta_2O_7$.

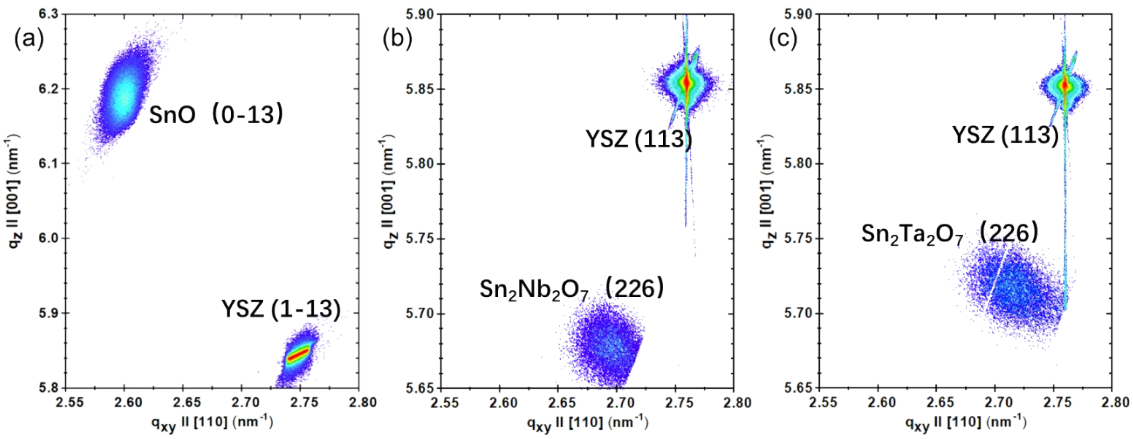

Figure S2. Reciprocal space mapping (RSM) of (a) SnO, (b) $Sn_2Nb_2O_7$ and (c) $Sn_2Ta_2O_7$ thin films grown on YSZ (001) substrate.

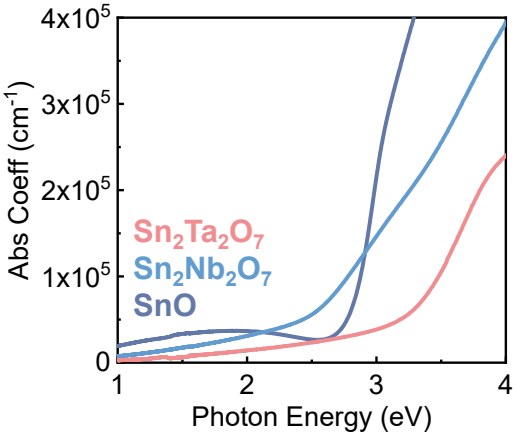

Figure S3. The optical absorption coefficient spectra of SnO, $Sn_2Nb_2O_7$ and $Sn_2Ta_2O_7$ thin films.

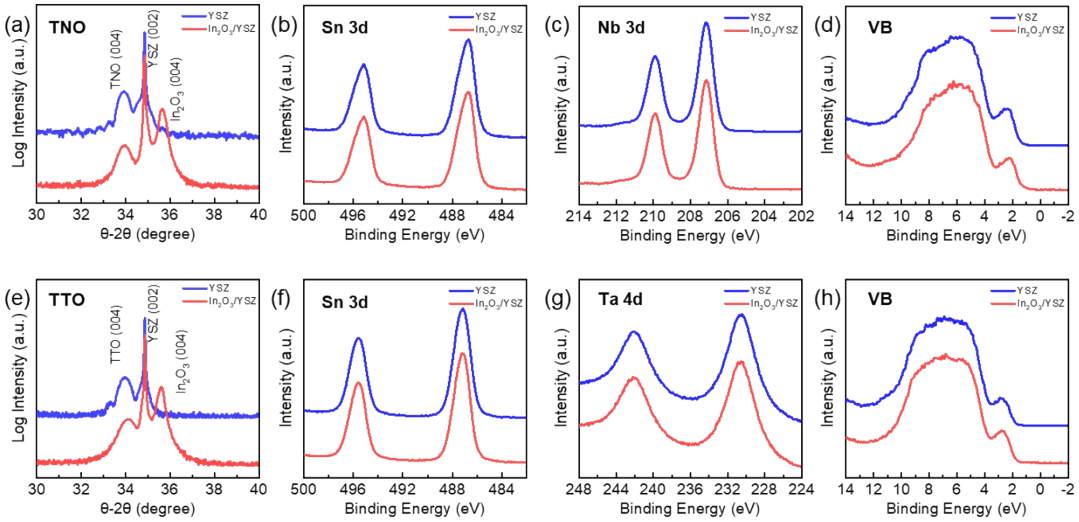

Figure S4. (a) X-ray diffraction (XRD) of $Sn_2Nb_2O_7$ (TNO) grown on YSZ (001) and In_2O_3 thin film coated YSZ(001) substrates; (b) Sn $3d_{5/2}$, (c) Nb 3d and (d) VB XPS spectra of TNO thin films excited with photon energy of 1486 eV; (e) X-ray diffraction (XRD) of $Sn_2Ta_2O_7$ (TTO) grown on YSZ (001) and In_2O_3 thin film coated YSZ (001) substrates; (b) Sn $3d_{5/2}$, (c) Nb 3d and (d) VB XPS spectra of TTO thin films excited with photon energy of 1486 eV.

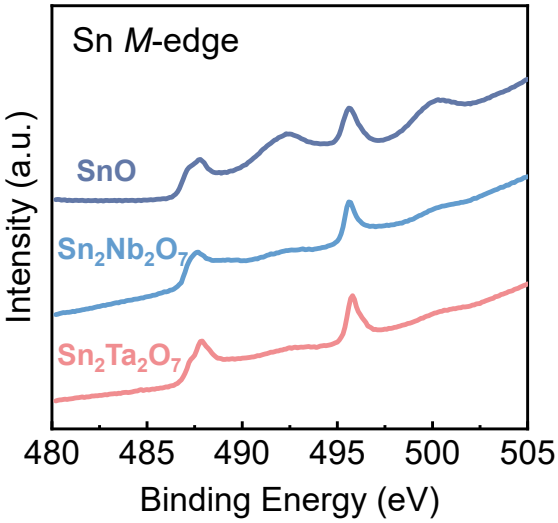

Figure S5. Sn M-edge XAS of SnO, $Sn_2Nb_2O_7$ and $Sn_2Ta_2O_7$.

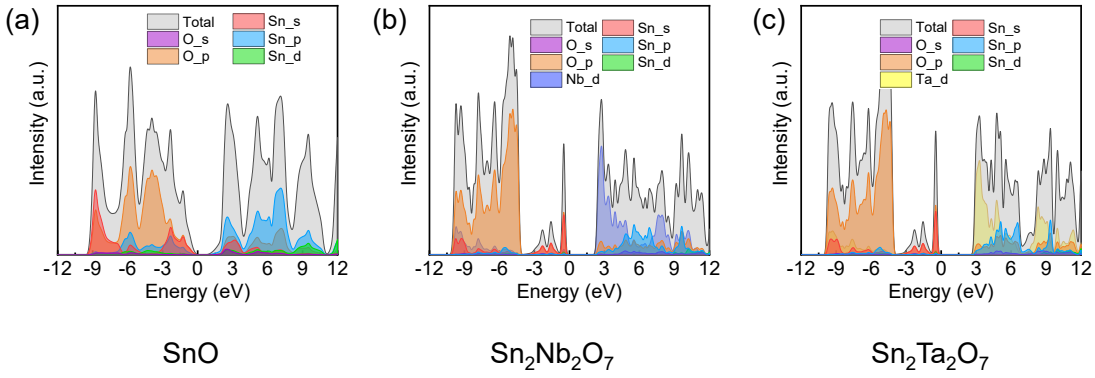

Figure S6. HSE06 calculated DOSs for (a) SnO, (b) $Sn_2Nb_2O_7$ and (c) $Sn_2Ta_2O_7$ from -12 eV to 12 eV.

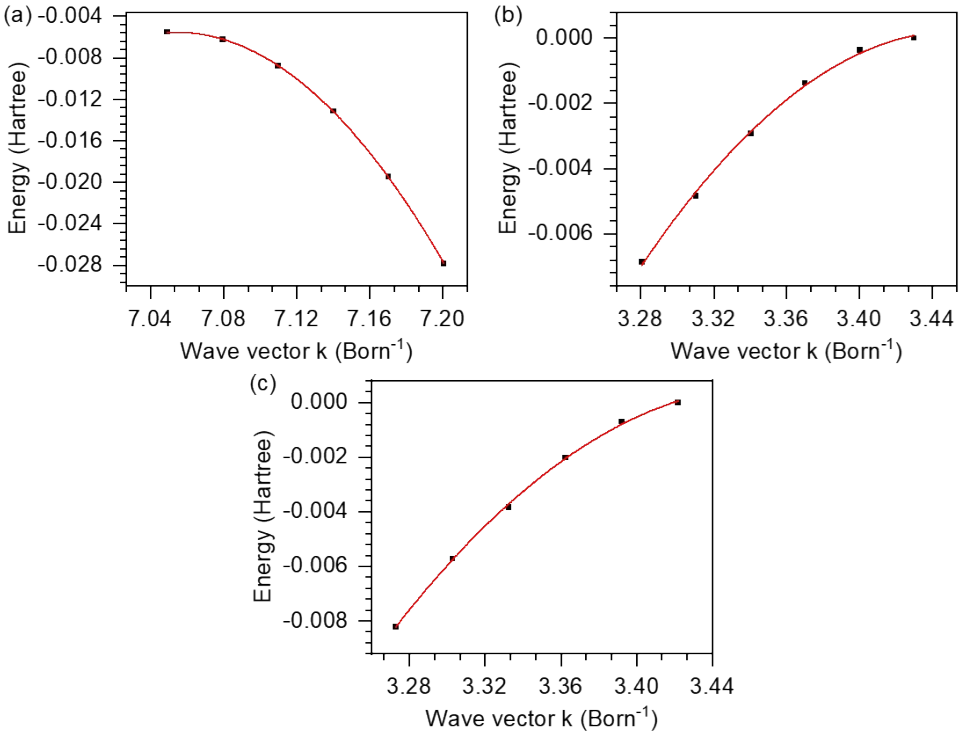

Figure S7. The parabolic fitting of hole effective mass at valence band maximum of (a) SnO; (b) $Sn_2Nb_2O_7$; (c) $Sn_2Ta_2O_7$.

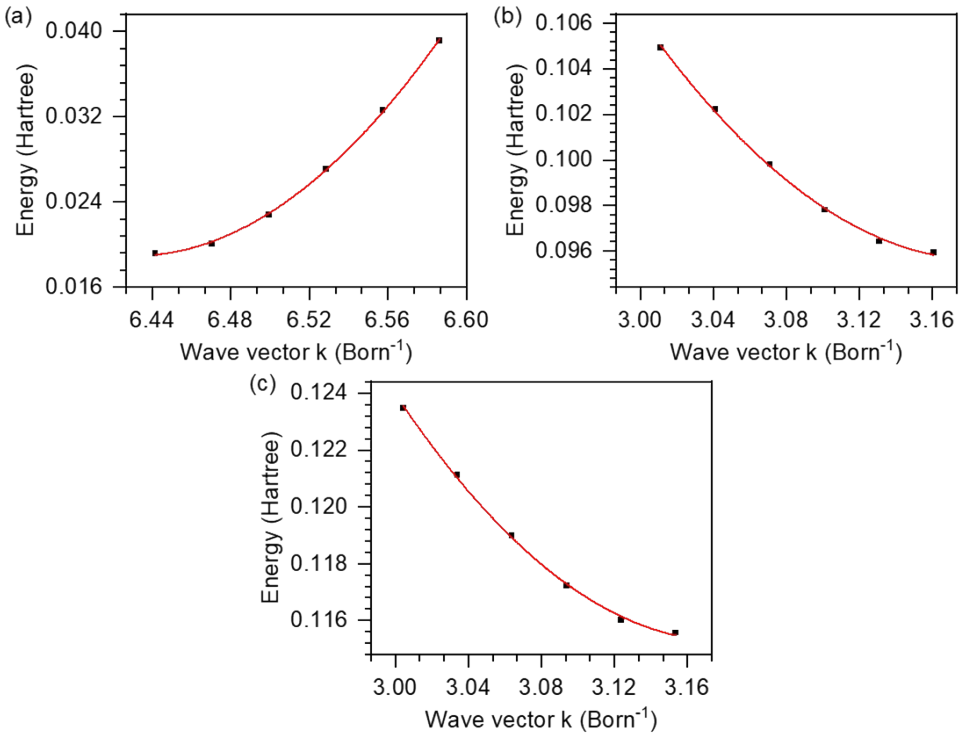

Figure S8. The parabolic fitting of electron effective mass at valence band maximum of (a) SnO; (b) $Sn_2Nb_2O_7$; (c) $Sn_2Ta_2O_7$.

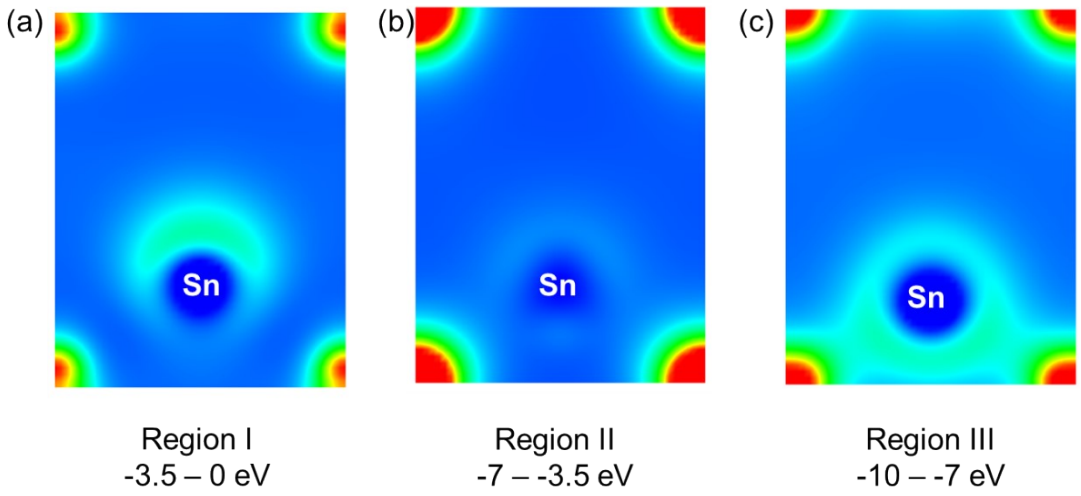

Figure S9. Partial electron density contour plots for litharge SnO. (a) -3.5 to 0 eV; (b) -7 to -3.5 eV (c) -10 to -7 eV.

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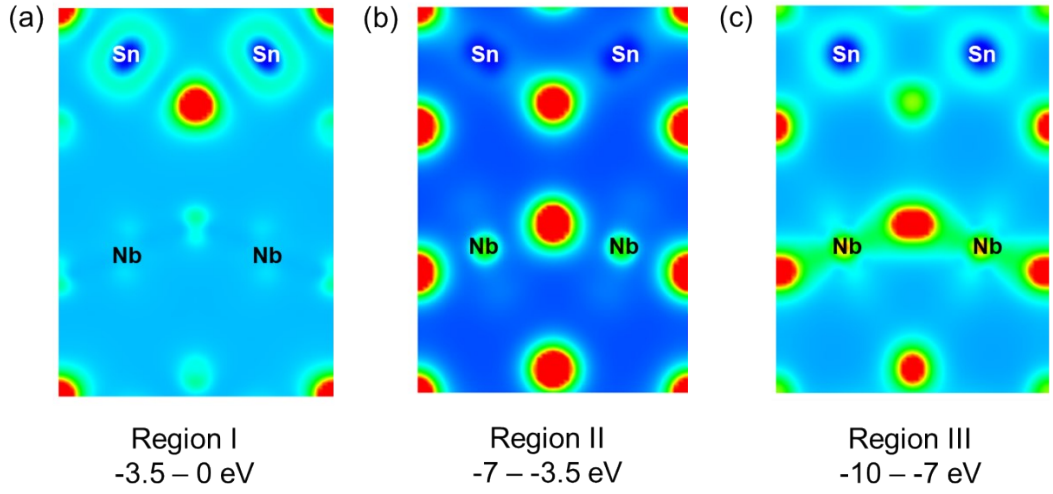

Figure S10. Partial electron density contour plots for pyrochlore $Sn_2Nb_2O_7$. (a) -3.5 to 0 eV; (b) -7 to -3.5 eV (c) -10 to -7 eV.

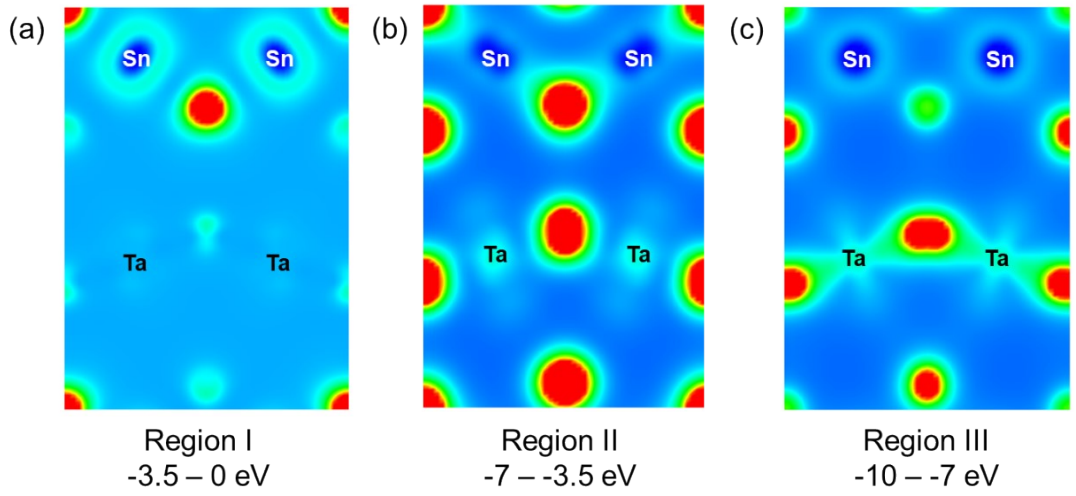

Figure S11. Partial electron density contour plots for pyrochlore $Sn_2Ta_2O_7$. (a) -3.5 to 0 eV; (b) -7 to -3.5 eV (c) -10 to -7 eV.

Table S1 The parabolic fitting parameters of hole effective mass

Materials	**Quadratic term coefficient (C) of fitting**	**Hole effective mass** $\frac{1}{2C} / m^*_{hole}$	**R-square (R^2) of fitting**	**Direction**
SnO (Tetragonal)	−1.008±0.013	0.496	0.9999	Γ−Z
$Sn_2Nb_2O_7$	−0.239±0.026	2.092	0.9983	Γ−L
$Sn_2Ta_2O_7$	−0.224±0.019	2.232	0.9993	Γ−L

Table S2 The parabolic fitting parameters of electron effective mass

Materials	**Quadratic term coefficient C of fitting**	**Electron effective mass** $\frac{1}{2C} / m^*_{elec}$	**R-square (R^2) of fitting**	**Direction**
SnO (Tetragonal)	0.624±0.098	0.801	0.9991	Γ−M
$Sn_2Nb_2O_7$	0.301±0.028	1.661	0.9988	Γ−K
$Sn_2Ta_2O_7$	0.265±0.026	1.887	0.9988	Γ−K

Table S3. Comparison of lattice parameters of epitaxial SnO, $Sn_2Nb_2O_7$ and $Sn_2Ta_2O_7$ thin films with their bulk values.

Materials	**In-Plane (Å)**	**Out-of-Plane (Å)**	**Bulk values (Å)**
SnO (Tetragonal)	a=3.84	c=4.85	a=3.80, c=4.84
$Sn_2Nb_2O_7$	a=10.49	a=10.57	a=10.58
$Sn_2Ta_2O_7$	a=10.42	a=10.49	a=10.48

Table S4. The parabolic fitted effective mass of electrons and holes at different k-points in the Brillion zone for SnO, $Sn_2Nb_2O_7$ and $Sn_2Ta_2O_7$. The directions of the carriers' movement are also listed behind the effective mass value.

Material		**Effective mass / m_e**	**Direction**
SnO	Electron	0.80	M-Γ
	Hole	0.50	Γ-Z
$Sn_2Nb_2O_7$	Electron	1.66	Γ-K
	Hole	2.09	L-Γ
$Sn_2Ta_2O_7$	Electron	1.89	Γ-K
	Hole	2.23	L-Γ