Supplementary Materials for "Microscopic Origin of Universal Quasi-Linear Band Structures of Transparent Conducting Oxides"

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Abstract

This supplementary information consists of the following 3 sections:

1. Pseudo-band structure of amophous In_2ZnO_4

2. Maximally Localized Wannier Functions of ZnO

3. Comparison of tight-binding results and first-principles calculations in the multicomponent and amorphous TCOs

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1. Pseudo-band structure of amophous In_2ZnO_4

In order to show that the band structure of the amorphous phases is not an artefact of the periodic boundary conditions, we compare band structures of the amorphous In_2ZnO_4 (a-IZO) with different cell dimension along a specific direction. The unit geometry is $11\times11\times11$ $Å^3$ cell containing 84 atoms in total. Then the lattice parameter is expanded by two or three times along the x-direction with proportionately larger number of atoms. [See Fig. 1(a).] Note that the melt-quench simulations were performed independently for each supercell. The band structure was computed along k_x and they were plotted in Fig. 1(b). For the multiplied supercells, the band structures were unfolded to match with the smallest supercell. (The conduction bottom is set to zero.) It is found that the dispersion is similar among all conduction bands except for the gap opening at the zone boundary points.

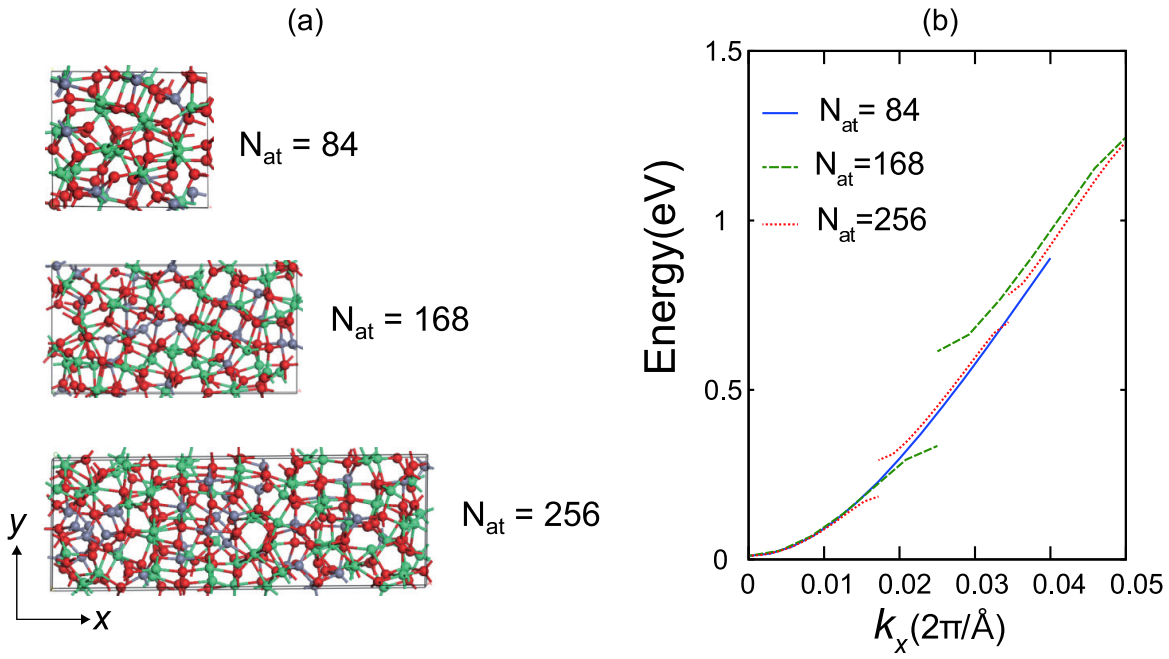

FIG. 1. (Color online) (a) a-IZO with different lattice parameters and numbers of atoms. (b) The conduction bands of a-IZO in (a). The bands for larger supercells are unfolded.

2. Maximally Localized Wannier Functions of ZnO

The maximally localized Wannier functions (MLWFs) for the zincblende ZnO were obtained by using the Quantum Espresso package [1] with wannier90 [2]. We consider 16 bands (9 bands are valence). Figure 2 shows constructed MLWFs except for Zn-d like MLWFs. (a), (b), and (c) resemble metal s, oxygen s, and the oxygen p_x orbitals, respectively. There are two more MLWFs that are similar to oxygen p_y and p_z orbtials.

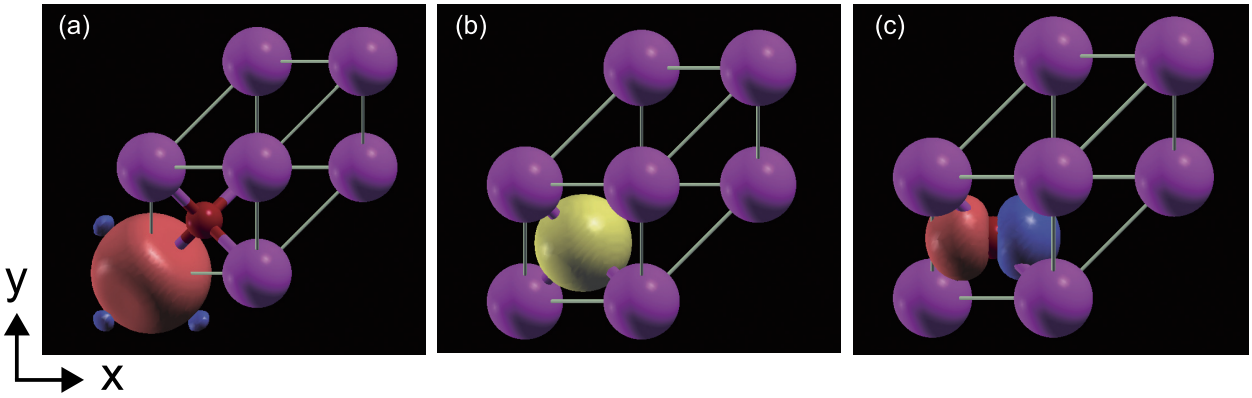

FIG. 2. (Color online) MLWFs in the zincblende ZnO. The large (small) spheres indicate Zn (O) atoms.

3. Comparison of tight-binding results and first-principles calculations in the multicomponent and amorphous TCOs

We compared TB results and GGA+U calculations for the crystalline In_2O_3, SnO_2, Zn_2SnO_4 and amorphous In_2ZnO_4 in Fig. 3. The notations in the figures are identical to those in Figs. 3(a) and 3(b) in the main text. The fitted parameters for various TCOs are compiled in Table I.

[1] S. Baroni *et al*, http:\\www.pwscf.org.

[2] A. A. Mostofi *et al*, http:\\www.wannier.org.

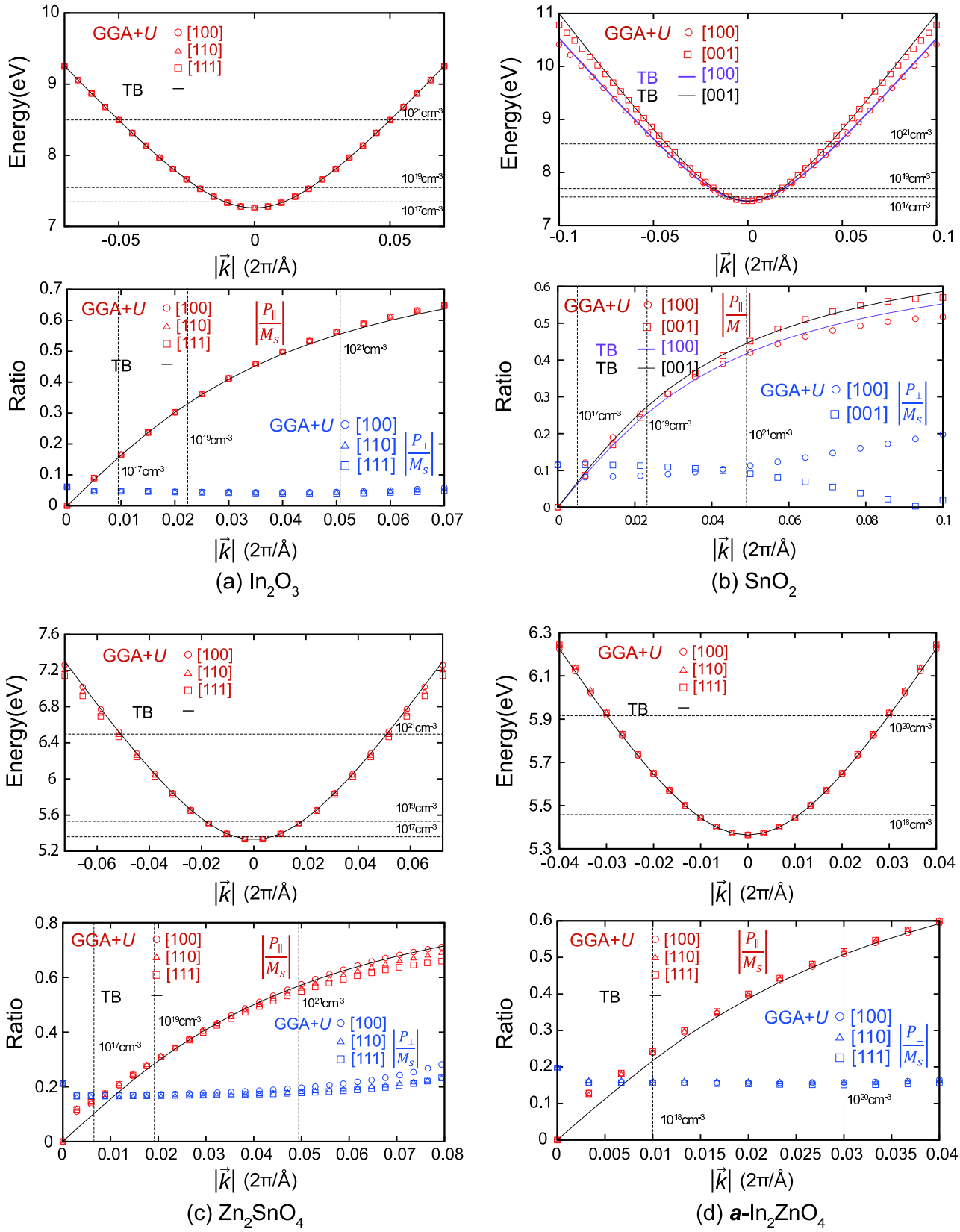

FIG. 3. (Color online). Band structures for various TCOs computed with GGA+U methods (discrete symbols). The fitting to the TB model is represented by solid lines.

TABLE I. The parameters in the TB model obtained by fits to the first-principles band structures within the GGA+U method. We used $E = \epsilon_0 + \sqrt{\epsilon^2 + \tilde{\gamma}^2 k^2}$ in which ϵ_0 means the energy separation between the valence top and the Dirac point. The effective mass (m_e^*) is calculated at the Γ point.

Materials	ϵ_0 (eV)	ϵ (eV)	$\tilde{\gamma}/\hbar(\times 10^5 m/s)$	m_e^*/m_e
ZnO	0.79	1.01	8.87	0.23
In_2O_3	0.66	1.17	10.16	0.20
SnO_2 [100]	0.15	1.22	9.95	0.22
SnO_2 [001]	0.14	1.20	11.37	0.19
Zn_2SnO_4	0.76	1.49	10.58	0.24
a-In_2ZnO_4	0.12	0.80	8.80	0.18
c-$InGaZnO_4$	0.85	1.55	10.42	0.25
a-$InGaZnO_4$	0.83	0.66	7.28	0.22