Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for:

Band Alignment and Charge Transfer Predictions of ZnO/ZnX (X = S, Se, Te) Interfaces Applied to Solar Cells: A PBE+U Theoretical Study

Efracio Mamani Flores,[†,‡] Rogério Almeida Gouvea,[†,‡] Maurício Jeomar Piotrowski,[†] and Mário L. Moreira.[*,†]

Department of Physics, Federal University of Pelotas, P.O. Box 354, 96010 900, Pelotas, RS, Brazil

E-mail: mlucio3001@gmail.com

[*]To whom correspondence should be addressed
[†]Department of Physics, Federal University of Pelotas, P.O. Box 354, 96010 900, Pelotas, RS, Brazil
[‡]Contributed equally to this work

1 Convergence Tests for ZnX (X = O, S, Se, Te)

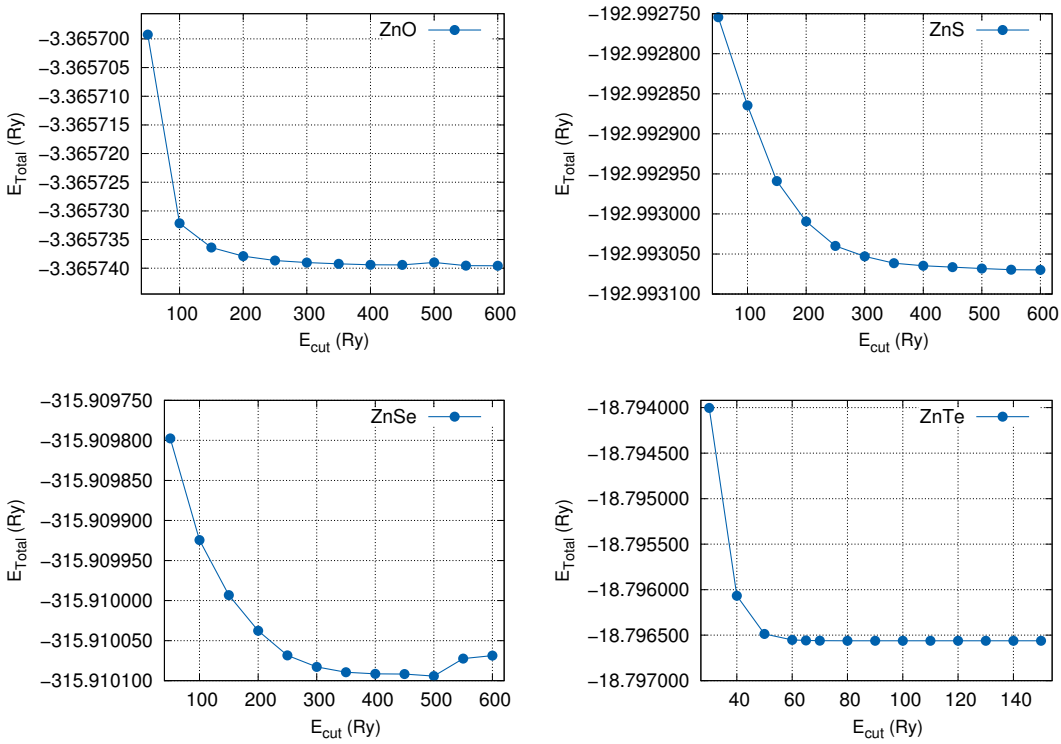

Figure S1: Convergence tests for ZnX *bulk*-like, total energy with respect to the cut-off energy (E_{cut}).

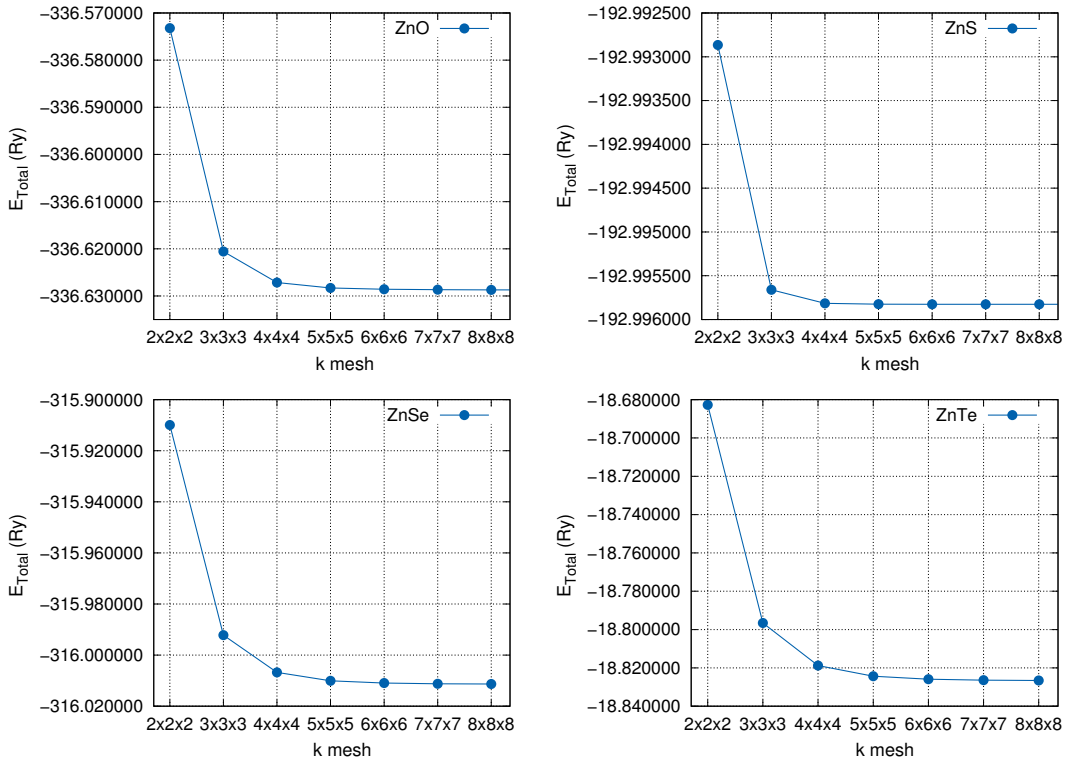

Figure S2: Convergence tests for ZnX *bulk*-like, total energy with respect to the **k**-points (**k**-mesh).

2 The Electronic Band Structure, the Total, and Partial Density of States (DOS) for ZnX (X = S, Se, Te) within PBE and PBE+U

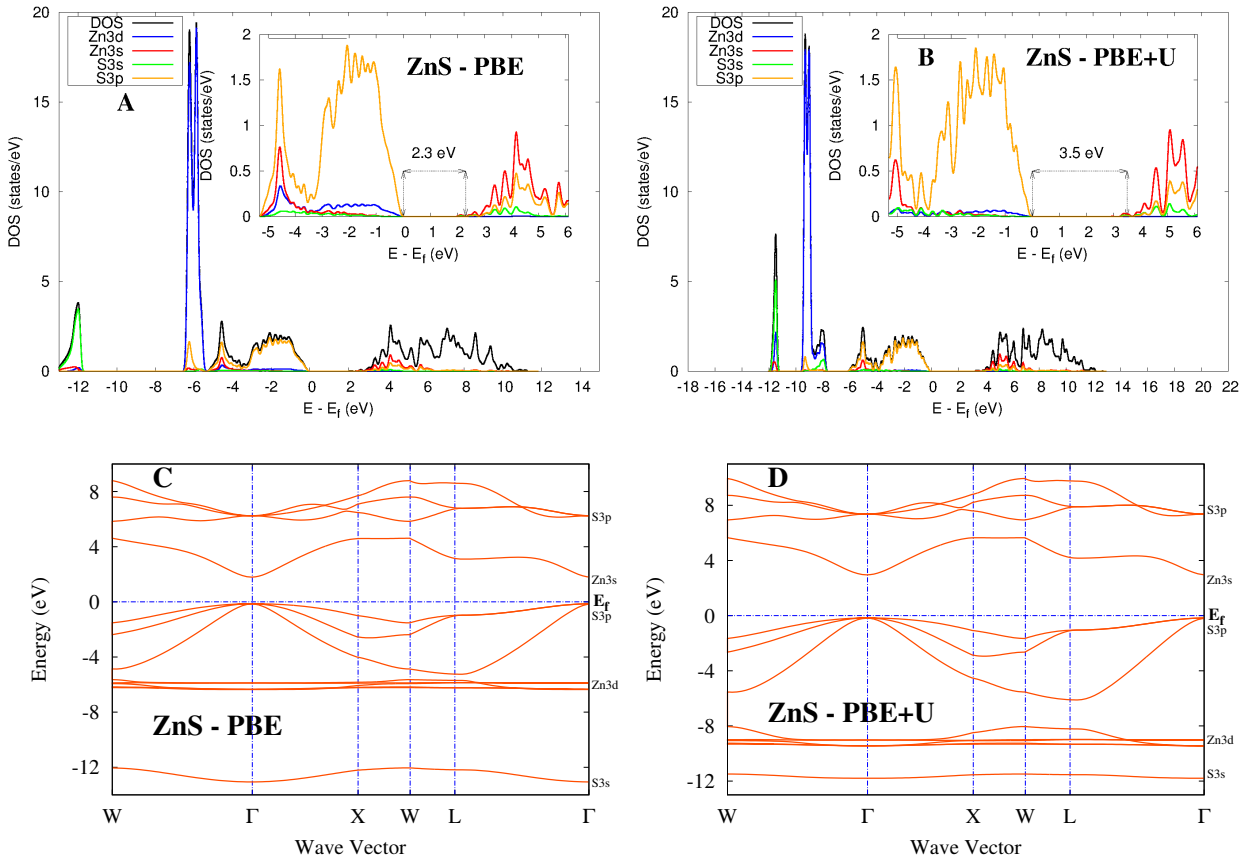

Figure S3: Total and partial density of states (DOS) for the *bulk* ZnS: **A** without Hubbard correction, **B** with Hubbard correction. Band structures for the *bulk* ZnS along with the high-symmetry points of the Brillouin zone: **C** without Hubbard correction, **D** with Hubbard correction.

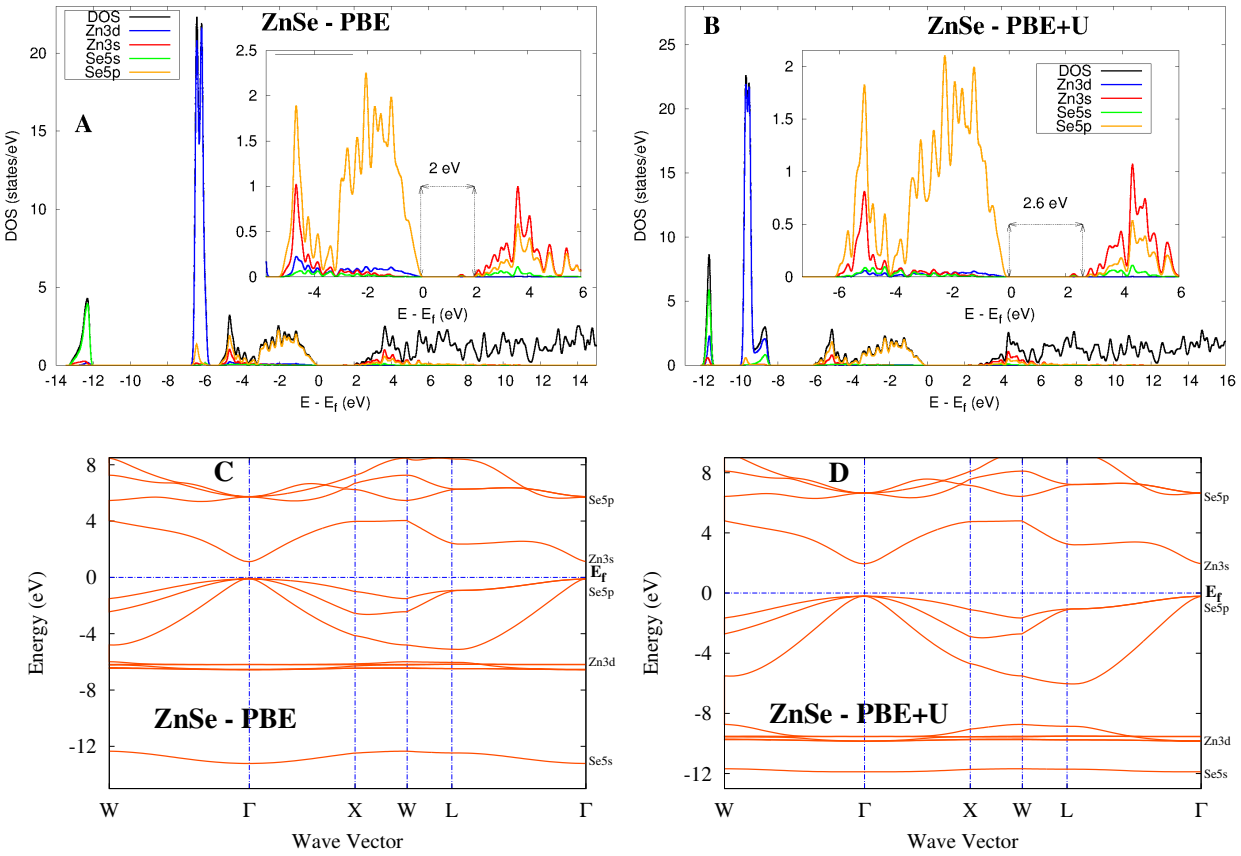

Figure S4: Total and partial density of states (DOS) for the *bulk* ZnSe: **A** without Hubbard correction, **B** with Hubbard correction. Band structures for the *bulk* ZnSe along with the high-symmetry points of the Brillouin zone: **C** without Hubbard correction, **D** with Hubbard correction.

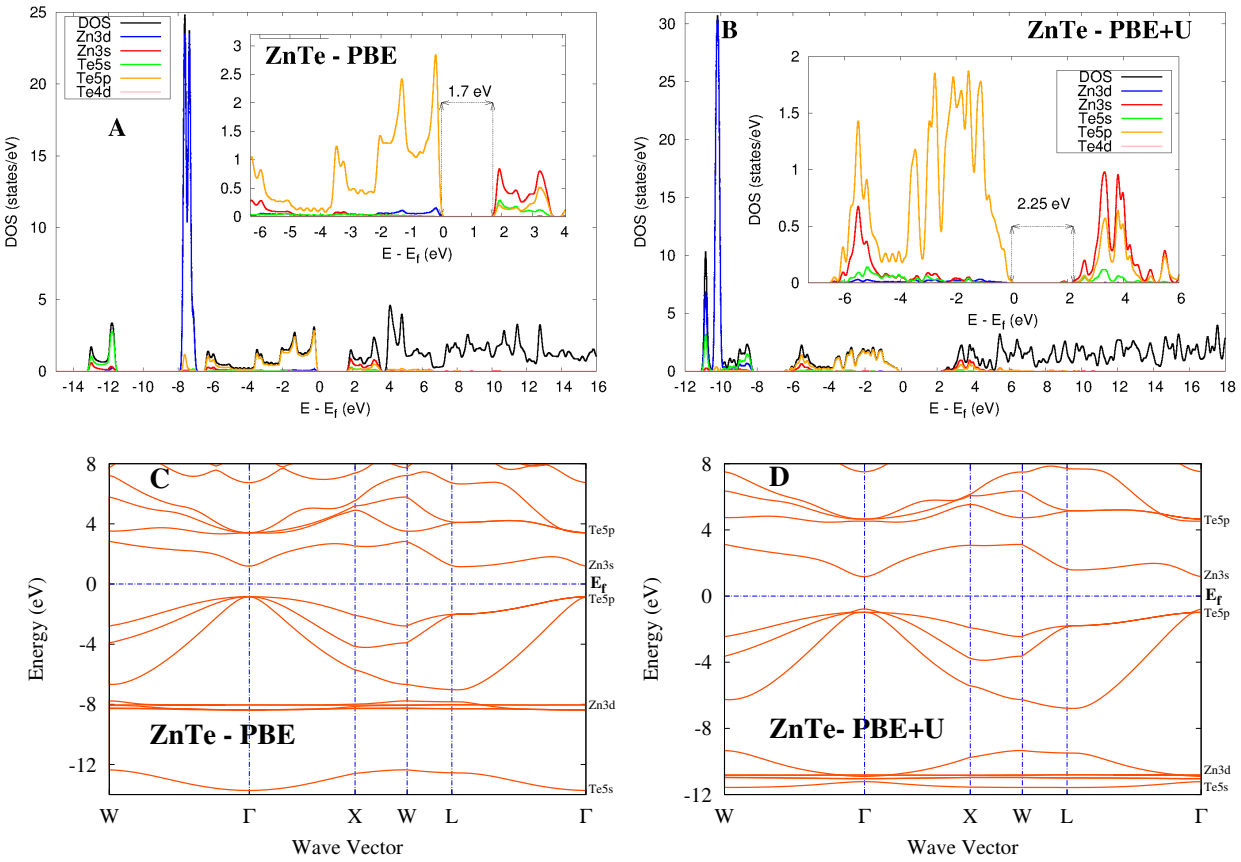

Figure S5: Total and partial density of states (DOS) for the *bulk* ZnTe: **A** without Hubbard correction, **B** with Hubbard correction. Band structures for the *bulk* ZnTe along with the high-symmetry points of the Brillouin zone: **C** without Hubbard correction, **D** with Hubbard correction.

3 The Total Density of States (PDOS) for Bulk ZnX (X = O, S, Se, Te) Using Hybrid Exchange-Correlation Functional

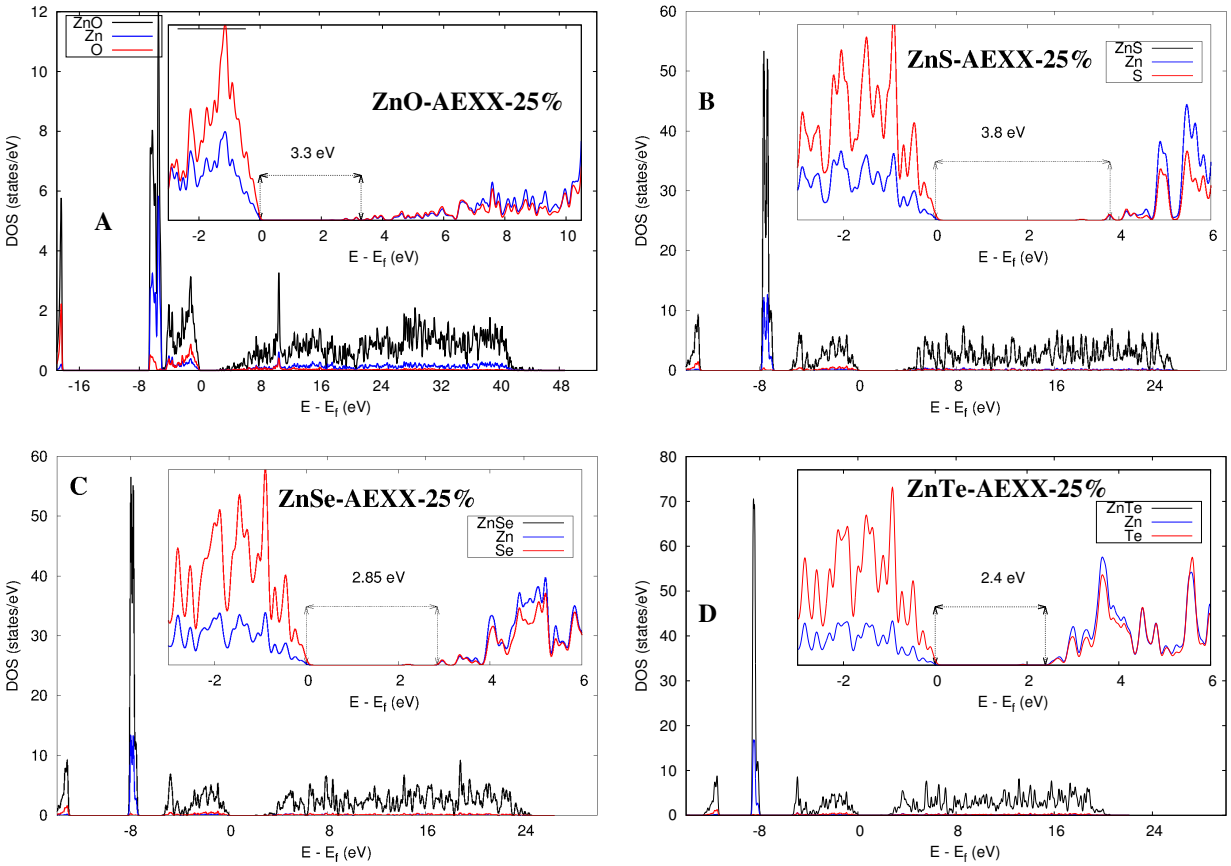

Figure S6: Total density of states (DOS) using a hybrid exchange-correlation functional (Heyd-Scuseria-Ernzerhof), with 25% of exact exchange, for: **A** ZnO, **B** ZnS, **C** ZnSe, and **D** ZnTe.

4 Interface ZnO/ZnTe

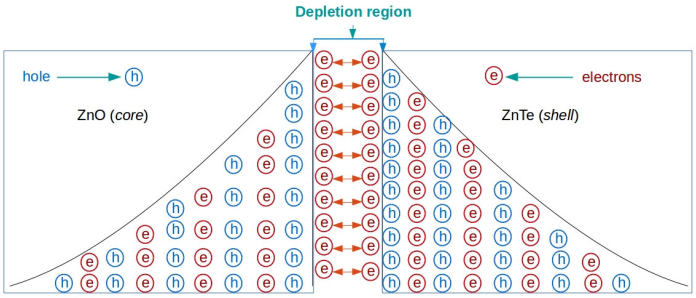

Figure S7: Illustrative scheme of the Schottky barrier in the interface ZnO/ZnTe.