Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Understanding the mechanism of enhanced charge separation and visible light photocatalytic activity of modified wurtzite ZnO with nanoclusters of ZnS and graphene oxide: from a hybrid density functional study

Francis Opoku[a], Krishna Kuben Govender[b], Cornelia Gertina Catharina Elizabeth van Sittert[c], Penny Poomani Govender[a,*]

[a] Francis Opoku

Department of Applied Chemistry, University of Johannesburg, P. O. Box 17011, Doornfontein Campus, 2028, Johannesburg, South Africa

Email: ofrancis2010@gmail.com

[b] Krishna Kuben Govender

Council for Scientific and Industrial Research, Meraka Institute, Center for High Performance Computing, 15 Lower Hope Road, Rosebank, Cape Town, 7700, South Africa

Email: kgovender@csir.co.za

[c] Cornelia Gertina Catharina Elizabeth van Sittert

Research Focus Area for Chemical Resource Beneficiation: Laboratory of Applied Molecular Modelling, North-West University, Potchefstroom, 2520, South Africa

Email: cornievansittert@nwu.ac.za

*Corresponding author: Penny Poomani Govender

Department of Applied Chemistry, University of Johannesburg, P. O. Box 17011, Doornfontein Campus, 2028, Johannesburg, South Africa

Email: pennyg@uj.ac.za

Tel: +27 11 559 6555

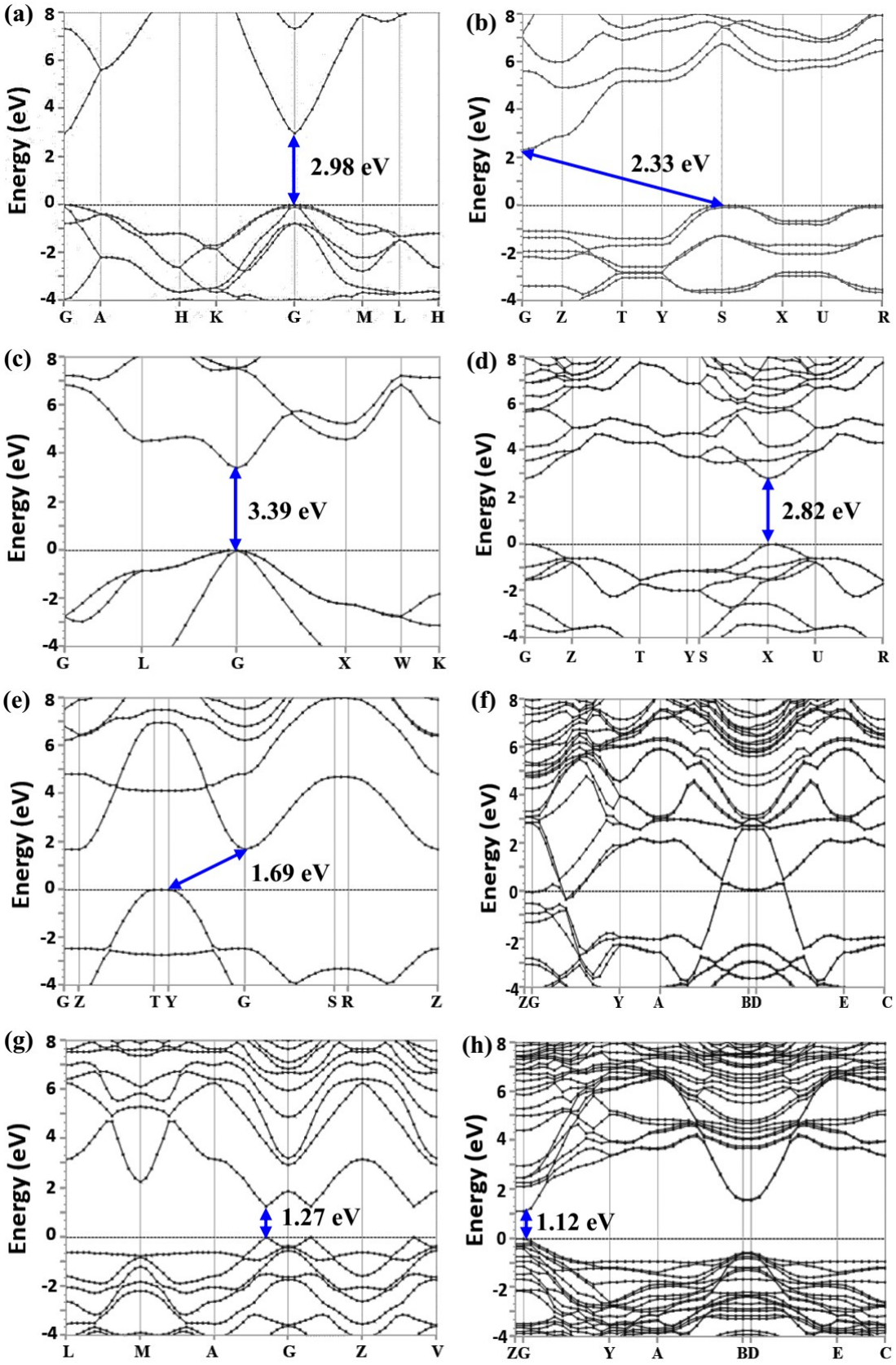

Fig. S1 GGA-PBE calculated band structures of (a) Pure ZnO, (b) ZnO(001), (c) Pure ZnS, (d) ZnS(110), (e) GO sheet, (f) ZnS(110)/GO (g) GO/ZnO(001) and (h) ZnS(110)/GO/ZnO(001) heterostructures.

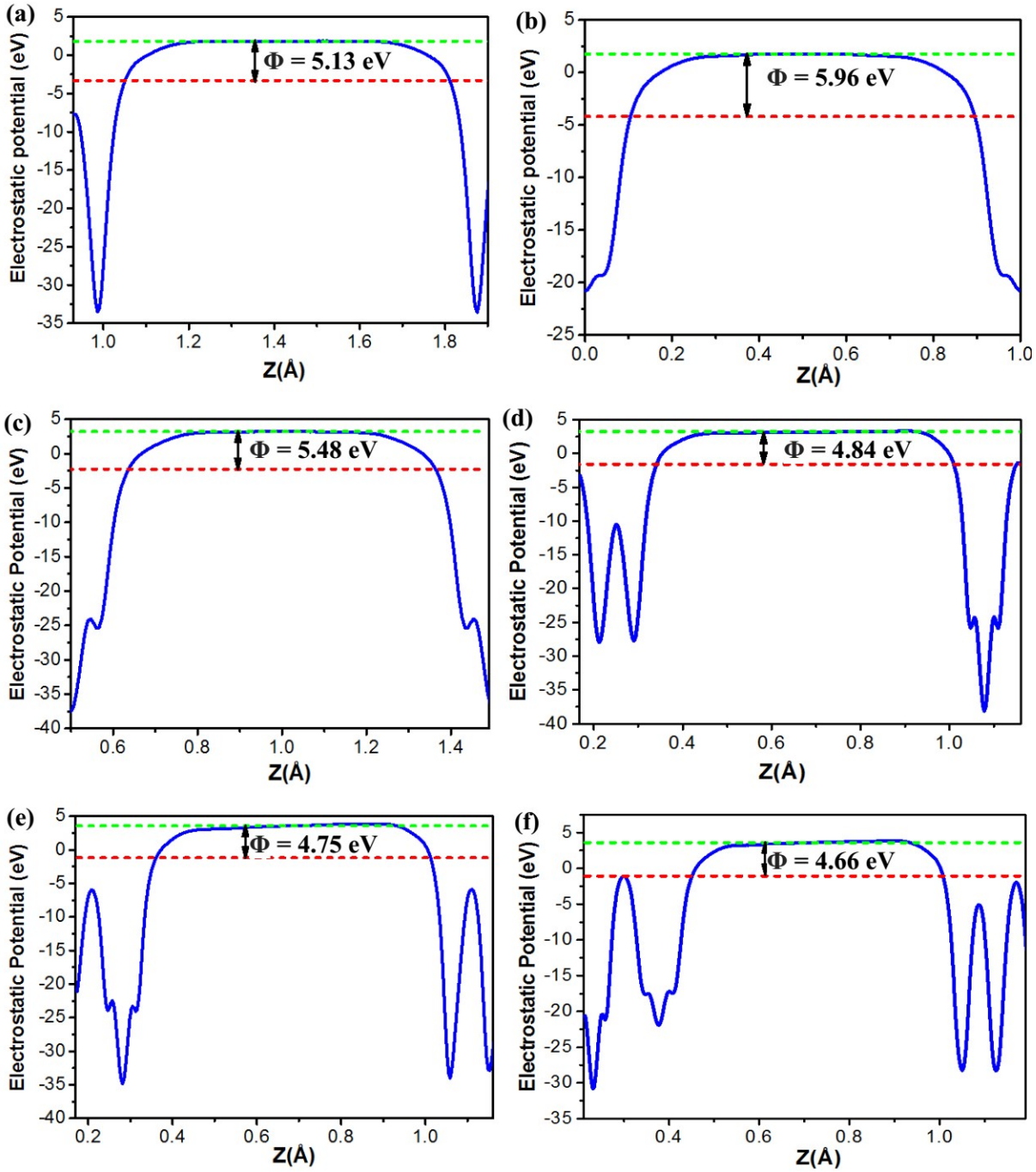

Fig. S2 Calculated electrostatic potentials for (a) ZnO, (b) ZnS, (c) GO sheet, (d) ZnS(110)/GO, (e) GO/ZnO(001) and (f) ZnS/GO/ZnO(001) within the GGA-PBE functional. The red and green dashed lines denote the Fermi level (E_F) and the vacuum energy (E_{vac}) level, respectively.