



Conejeros, S., Allan, N., Hart, J., & Claeysens, F. (2019). Graphene and novel graphitic ZnO and ZnS nanofilms: the energy landscape, non-stoichiometry and water dissociation. *Nanoscale Advances*, 1(5), 1924-1935. <https://doi.org/10.1039/C8NA00155C>

Publisher's PDF, also known as Version of record

License (if available):  
CC BY

Link to published version (if available):  
[10.1039/C8NA00155C](https://doi.org/10.1039/C8NA00155C)

[Link to publication record on the Bristol Research Portal](#)  
PDF-document

This is the final published version of the article (version of record). It first appeared online via RSC at <https://pubs.rsc.org/en/content/articlelanding/2019/NA/C8NA00155C#!divAbstract> . Please refer to any applicable terms of use of the publisher.

## University of Bristol – Bristol Research Portal

### General rights

This document is made available in accordance with publisher policies. Please cite only the published version using the reference above. Full terms of use are available: <http://www.bristol.ac.uk/red/research-policy/pure/user-guides/brp-terms/>

## Supporting information

### **Graphene and novel graphitic ZnO and ZnS nanofilms: the energy landscape, non-stoichiometry and water dissociation**

Sergio Conejeros\*<sup>a,b</sup>, Neil L. Allan<sup>a</sup>, Frederik Claeysens<sup>c</sup> and Judy N. Hart<sup>d</sup>

<sup>a</sup>School of Chemistry, University of Bristol, Cantock's Close, Bristol, U.K., BS8 1TS.

<sup>b</sup>Departamento de Química, Universidad Católica del Norte, Av. Angamos 0610, Antofagasta, Chile, 124000.

<sup>c</sup>Department of Engineering Materials, University of Sheffield, Sir Robert Hadfield Building, Mappin Street, Sheffield S1 3JD

<sup>d</sup>School of Materials Science & Engineering, UNSW Sydney, NSW 2052 Australia

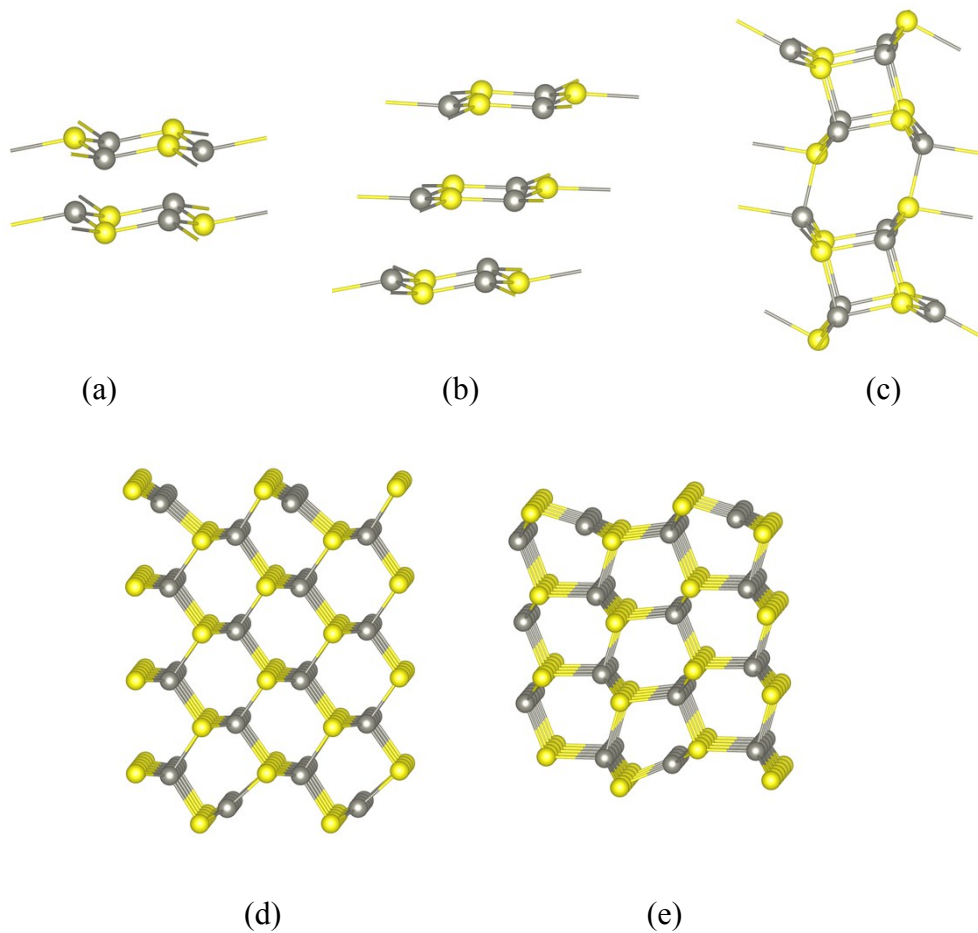


Figure S1. Optimised structures of those ZnS films where there is substantial structural relaxation from the ideal structures shown in Figure 1: a) Eclipsed graphitic (2 layers), b) Staggered graphitic (3 layers), c) non-polar BCT, d) non-polar ZB(110) and e) non-polar WZ( $10^{10}$ ). Zn atoms are grey, S yellow.

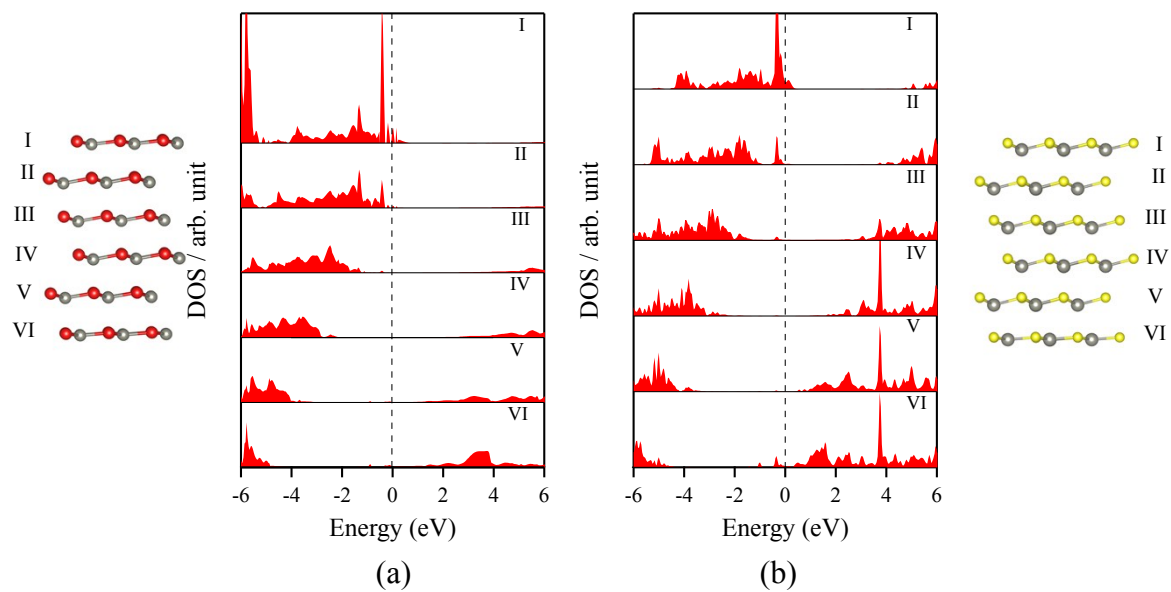


Figure S2. Partial density of states (PDOS) per layer for polar ZB(111) films with 6 layers for a) ZnO and b) ZnS. Corresponding structures are shown beside the DOS. The vertical dashed line indicates the Fermi level.

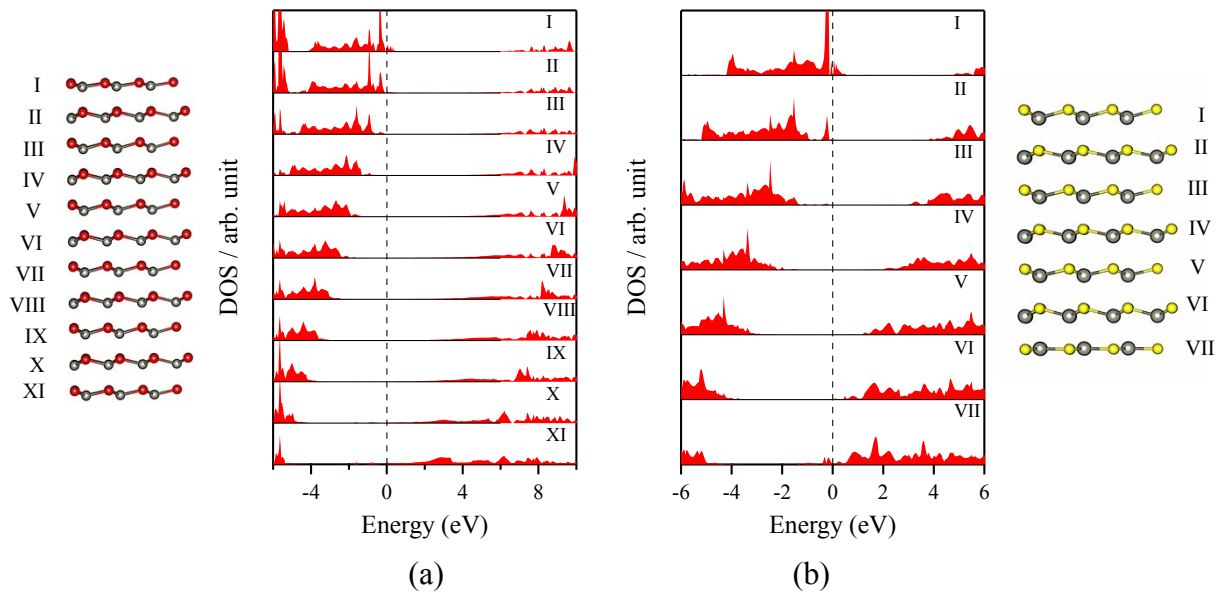


Figure S3. Partial density of states (PDOS) per layer for polar WZ(0001) films for a) ZnO with 11 layers and b) ZnS with 7 layers (the smallest thicknesses for which these structures are stable). Corresponding structures are shown beside the DOS. The vertical dashed line indicates the Fermi level.

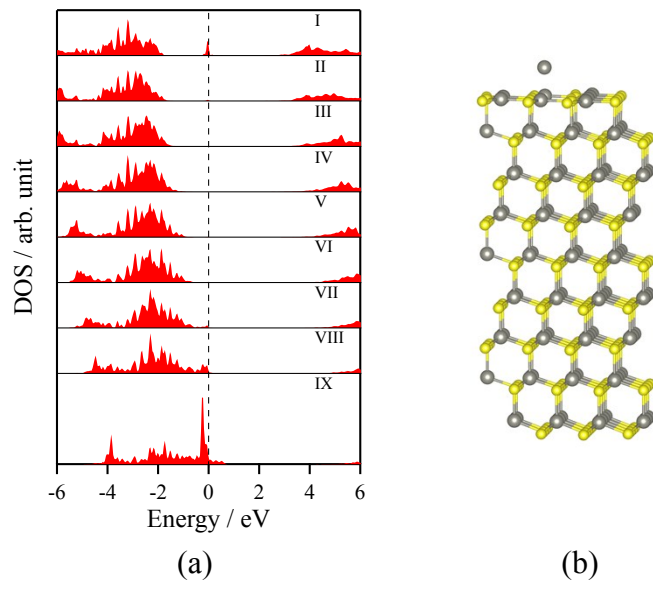


Figure S4. Partial density of states (PDOS) per layer for polar ZB(111) for ZnS with 9 layers.