THE JOURNAL OF PHYSICAL CHEMISTRY C

Addition/Correction

pubs.acs.org/JPCC

Correction to "Structures, Energetics, and Electronic Properties of Layered Materials and Nanotubes of Cadmium Chalcogenides"

Jia Zhou,* Jingsong Huang, Bobby G. Sumpter, Paul R. C. Kent, Humberto Terrones, and Sean C. Smith

J. Phys. Chem. C **2013**, *117* (48), 25817−25825. DOI: 10.1021/jp409772r

We have recently become aware of a published paper titled "Two-Dimensional CdSe Nanosheets and Their Interaction with Stabilizing Ligands" by X.-D. Wen, R. Hoffmann, and N. W. Ashcroft.[1] Given the relevance and contextual similarities to our paper, this erratum acknowledges our oversight and provides brief details highlighting how the two studies offer valuable and original results.

In the paper by Wen, Hoffmann, and Ashcroft, the stability of graphene-like 2D single-layer (SL) sheets sheet of CdSe with and without ligands is studied using density functional theory. They found that 2D SL sheets without ligands display a nearly planar graphene-like lattice, similar to what we have found in our work. Moreover, they also studied four ways of assembling 3D structures by stacking the SL sheets. However, they examined the eclipsed geometry with an AA or AB stacking sequence, the latter of which collapsed to the 3D bulk wurtzite structure, whereas we proposed multilayer (ML) stacks with a staggered geometry and an AB stacking sequence as in graphite, which collapsed to a new phase different from the bulk wurtzite or zinc blend structures. Their studies on the 2D CdSe sheet protected with ligands are closely relevant to experimental syntheses of stable 3D crystals of 2D sheets of ZnS, ZnSe, ZnTe, and CdSe, stabilized by a variety of alkylamines.

Our paper mainly dealt with various possible structures of cadmium chalcogenides, CdX (X = S, Se, Te), including free-standing 2D SL sheets, 3D ML stacks, and 1D nanotubes. In addition to the structures and stabilities of the proposed materials, we also studied their electronic structures, especially the band gaps relevant to photovoltaics by the state-of-the-art GW approach. These new structures are found to be complementary to the bulk zinc blend and wurtzite materials, allowing a much wider wavelength range on the spectrum, from infrared, visible, to ultraviolet, to be utilized. Through these theoretical studies, new members of free-standing CdX are introduced into the family of 2D inorganic graphene analogues that could be of considerable interest for future experimental studies.

REFERENCES

(1) Wen, X.-D.; Hoffmann, R.; Ashcroft, N. W. Two-Dimensional CdSe Nanosheets and Their Interaction with Stabilizing Ligands. *Adv. Mater.* **2013**, *25*, 261−266.

Published: December 6, 2013