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EXPRESSION OF CONCERN

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Expression of concern: Surface-dependent band structure variations and bond deviations of GaN

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Expression of concern for 'Surface-dependent band structure variations and bond deviations of GaN' by Chih-Shan Tan *et al.*, *Phys. Chem. Chem. Phys.*, 2022, **24**, 9135–9140, **https://doi.org/10.1039/D2CP00100D**.

The Royal Society of Chemistry has been contacted by a reader who raised concerns about the computational methodology applied in this work, and suggested that the nature of the calculations meant that the results would have no physical meaning.

We consulted an independent expert who agreed with the concerns and said that the authors did not introduce a vacuum layer, which is needed to model the surface of a material. They added that as a result, their calculations have no physical meaning in terms of providing a description of any surface.

The authors dispute these concerns, and have provided the following statement:

This work was conducted to provide some explanation of the observation of facet-dependent electrical conductivity properties of commercially available GaN wafers (*J. Mater. Chem. C*, 2021, **9**, 15354). The {0001} face of a GaN wafer is much more conductive than its {10−10} face. To us, the most important result of the DFT calculations is to show that there are bond length variations and bond distortions within the surface planes of GaN. These small positional deviations in surface atoms may exist, so the prediction provided by the calculations is useful in this regard. Of course, it is not realistic to think there are periodic variations in band gaps. Readers should know this is not physical reality. As for the criticism of not introducing a vacuum layer to model the surface of a material, Dr Tan argues that GaN crystals and wafers are not produced in a vacuum, but through a high-temperature Czochralski process in the case of wafers. This is why we set no vacuum layer in the slab as the surface layer. From our point of view, the atomic model of the surface of a single crystal depends on the real crystal growth conditions, as the purpose of the calculations is to explain experimental observations. We would like to see publications using better DFT approaches to explain the various facet-dependent properties of semiconductor crystals.

The independent expert felt that this response did not sufficiently address the concerns that have been raised. They said that regardless of how the surfaces are produced and whether they are exposed to a vacuum or atmosphere, a slab model must be used to model a surface. If 2D slabs are not separated by a vacuum, as in the present work, one is modeling a bulk material and not a surface. There are many DFT studies in the literature, all of which use slabs separated by vacuum layers, to model surfaces.

Physical Chemistry Chemical Physics is publishing this Expression of Concern to inform readers that we are unable to confirm the accuracy of the conclusions reported in this paper.

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