INORGANIC CHEMISTRY
FRONTIERS

EXPRESSION OF CONCERN





Cite this: *Inorg. Chem. Front.*, 2022, **9**, 4836

# Expression of concern: Surface-dependent band structure variations and bond-level deviations in $Cu_2O$

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DOI: 10.1039/d2qi90061k
rsc.li/frontiers-inorganic

Expression of concern for 'Surface-dependent band structure variations and bond-level deviations in $Cu_2O$' by Chih-Shan Tan and Michael H. Huang, *Inorg. Chem. Front.*, 2021, **8**, 4200–4208, **https://doi.org/10.1039/D1QI00733E**.

The Royal Society of Chemistry has been contacted by a reader who informed us there were errors in the computational methodology applied in this work; the main concern is related to the fact that the geometry and band gap are reported to be unchanged with an increase in the number of layers in the 100 surface. As part of our investigation, we consulted with independent experts who also raised concerns over the methodology, describing it as fundamentally flawed on the basis that the slab models are identical to a supercell of the primitive cell, and therefore do not give information about the surfaces, concluding that the slabs in this paper have no physical meaning.

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

"This work uses the "find symmetry" function to give the unit of slab structure for subsequent calculations, which results in periodic variation in band gaps. The exchange–correlation function, BLYP, was set to consider only the effective core electron potential to obtain 1.787 eV for the band gap. So far it appears no DFT approach can truly address the facet-dependent properties of $Cu_2O$ crystals".

Inorganic Chemistry Frontiers is publishing this Expression of Concern to alert readers that we are presently unable to confirm the accuracy of the conclusions reported in this paper. An expression of concern will continue to be associated with the article until we receive conclusive evidence regarding the reliability of the reported data.

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11th August 2022
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