

# Author Correction: The first-principles phase diagram of monolayer nanoconfined water

<https://doi.org/10.1038/s41586-025-09872-5>

Published online: 2 December 2025

Correction to: *Nature* <https://doi.org/10.1038/s41586-022-05036-x>

Published online 14 September 2022



**Venkat Kapil, Christoph Schran, Andrea Zen, Ji Chen, Chris J. Pickard & Angelos Michaelides**

In the originally published version of this article, we incorrectly reported the total pressure applied to the full simulation cell ( $P_{\text{sim}}$ ) as the pressure experienced in the confined region of water. This is erroneous as the confinement pressure is higher and is approximated as  $P_{\text{conf}} = P_{\text{sim}} * z/w$ , where  $z$  is the  $z$ -dimension of the simulation box (assuming an  $x$ - $y$  confinement plane) while  $w$  is the confinement width<sup>1–3</sup>. Further details on estimating the pressure are in the updated Methods section. This correction does not affect the simulations or the observed phase behaviour, but it scales the pressure values by approximately a factor of 3. The onset of superionic behaviour occurs at 10.5–12 GPa rather than 3.5–4 GPa. Qualitative conclusions of the work remain unchanged. We also make an additional clarifying point that the statement on the impact of quantum nuclear effects on the phase transition only concerns the solid phases.

Text has been edited throughout the article; Figs. 1–3, Extended Data Figs. 1–5, Extended Data Tables 1–3, Source Data for Figs. 1 and 3 and Supplementary Videos 1–6 have been updated. The changes have been made in the HTML and PDF versions of the article. For comparison, the original, uncorrected article is available as Supplementary Information alongside this article.

1. Chen, J., Schusteritsch, G., Pickard, C. J., Salzmann, C. G. & Michaelides, A. Two dimensional ice from first principles: Structures and phase transitions. *Phys. Rev. Lett.* **116**, 025501 (2016).
2. Lin, B., Jiang, J., Zeng, X. C. & Li, L. (2023). Temperature-pressure phase diagram of confined monolayer water/ice at first-principles accuracy with a machine-learning force field. *Nat. Commun* **14**, 4110 (2023).
3. Jiang, J. et al. Rich proton dynamics and phase behaviours of nanoconfined ices. *Nat. Phys.* **20**, 456–464 (2024).

**Supplementary information** is available in the online version of this amendment.

© The Author(s), under exclusive licence to Springer Nature Limited 2025