Comment on “Two-Dimensional Boron Monolayer Sheets”

In a recent study, Wu et al. predicted that the $\alpha_1$-sheet boron monolayer is the most stable boron sheet using the PBE0 hybrid functional, instead of the previously predicted $\alpha$-sheet using the LDA and PBE functionals. However, their PBE0 cohesive energies are unreliable because the $k$-point sampling in the Brillouin zone is too coarse and the total energy is not variational with respect to the number of $k$-points.

Our calculations indicated that both the PBE and PBE0 cohesive energies of the $\alpha_1$-sheet are fluctuating as the $k$-point mesh increases from $3 \times 3 \times 1$ to $7 \times 7 \times 1$ (Figure 1) in the Monkhorst-Pack scheme. In the PBE0 calculations of ref 1, the Brillouin zone is sampled using $k$-points with 0.05 Å$^{-1}$ spacing, whose mesh should be $4 \times 4 \times 1$ or $5 \times 5 \times 1$ so that the total energy is not converged with respect to the $k$-point mesh. When the $k$-point mesh increases to $10 \times 10 \times 1$, the errors of cohesive energies of $\alpha$- and $\alpha_1$-sheets are less than 1 meV. As shown in Figure 1, the $\alpha$-sheet boron is more stable than the $\alpha_1$-sheet using the PBE0 and PBE functionals.

![Figure 1](image.png)

Figure 1. Convergence of cohesive energies of $\alpha$- and $\alpha_1$-sheet borons with respect to the $k$-point mesh using the PBE0 and PBE functionals.

All calculations were implemented in VASP5.2,5-6 package. The ion–electron interaction is treated using the projector-augmented wave (PAW)5,6 technique, and the plane-wave cutoff is set to 500 eV. The $\alpha$- and $\alpha_1$-sheets are optimized using the PBE functional, and the $k$-point mesh is $10 \times 10 \times 1$.

REFERENCES AND NOTES