Comment on "Two-Dimensional Boron Monolayer Sheets"

■ In a recent study, Wu *et al.*[1] predicted that the α_1-sheet boron monolayer is the most stable boron sheet using the PBE0 hybrid functional, instead of the previously predicted α-sheet[2] using the LDA and PBE functionals. However, their PBE0 cohesive energies are unreliable because the *k*-point sampling in the Brillioun zone is too coarse and the total energy is not variational with respect to the number of *k*-points.[3]

Our calculations indicated that both the PBE and PBE0 cohesive energies of the α_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 Brillioun 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 α- and α_1-sheets are less than 1 meV. As shown in Figure 1, the α-sheet boron is more stable than the α_1-sheet using the PBE0 and PBE functionals.

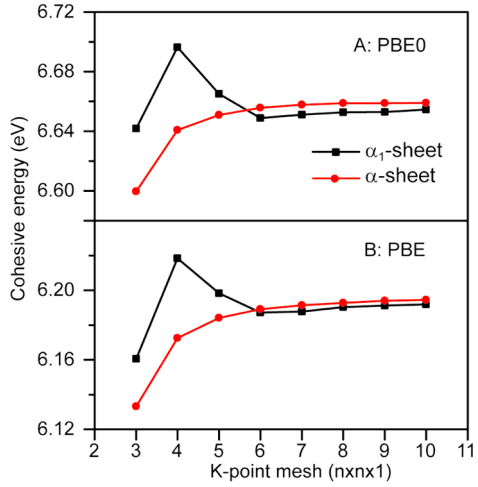

Figure 1. Convergence of cohesive energies of α- and α_1-sheet borons with respect to the *k*-point mesh using the PBE0 and PBE funcionals.

All calculations were implemented in VASP5.2[3,4] 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 α- and α_1-sheets are optimized using the PBE functional, and the *k*-point mesh is $10 \times 10 \times 1$.

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Received for review July 26, 2012

Published online February 26, 2013
10.1021/nn3033562