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In a recent letter, density functional theory (DFT) calculations were carried out on a structure observed by high resolution transmission electron microscopy experiments and used to predict that τ-B is the ground state structure of elemental boron at atmospheric pressure.[1] We have performed DFT total energy calculations on the structures provided in the Supplemental Material (SM) of ref [1] using the same code (VASP v.5.3.5) and calculation conditions used in that work and with two projector-augmented wave pseudopotentials distributed with the VASP code that have different core radius for the projection operator: RMAX = 2.583 (PS 1) and RMAX = 1.732 (PS 2).[2-5] In ref [1], it was reported that the pseudopotential from ref [5] was used for all calculations. An additional set of calculations were performed using PWSCF v5.2.0[6] with a cutoff energy of 40 Ry using an ultrasoft pseudopotential [7] and with a well converged numbers of k-points. The relative energies of our three independent calculations are all in agreement (within about 0.2 meV/atom) and indicate that τ-B106 is higher in energy than both α-B12 and β-B106 ($\delta E_{\tau-\alpha}$=+12.9 meV/atom, $\delta E_{\tau-\beta}$=+11.8 meV/atom), i.e. the ground state of elemental boron is not τ-boron. To understand the source of discrepancy between our results and the results presented in ref [1], we compared the total energies of these systems calculated with VASP, the code that was used to obtain the results of ref [1], using the two different pseudopotentials PS 1 and PS 2 (see Fig. 1). It has turned out that our total energies of τ-B105 and τ-B106 calculated with PS 2 are identical to the corresponding values reported in Table S1 of the SM of ref [1], while our total energies of α-B12, β-B105, β-B106, and γ-B28 calculated with PS 1 are identical to the corresponding values in the SM for ref [1] (Fig. 1). This observation strongly suggests that the total energies provided in the SM of ref [1] were obtained with two different pseudopotentials. Finally, we comment on the revised conclusions provided in the Erratum regarding relative stabilities of β-boron and τ-boron at high temperature. The claim that τ-boron may be more stable than β-boron for T>950K, is in contradiction with the experimental observation that liquid boron solidifies into β-boron, not τ-boron [8,9].

In summary, we have performed DFT total energy calculations of the boron allotrope structures published in ref [1] using two different ab-initio codes, VASP and PWSCF, and two different pseudopotentials for VASP. None of our simulation results support the conclusion of ref [1], and instead indicate that τ-boron is not the ground state. We have shown clear evidence that the total energies calculated with VASP and published in ref [1] were most likely obtained by the inconsistent use of pseudopotentials, which has led to an incorrect conclusion.

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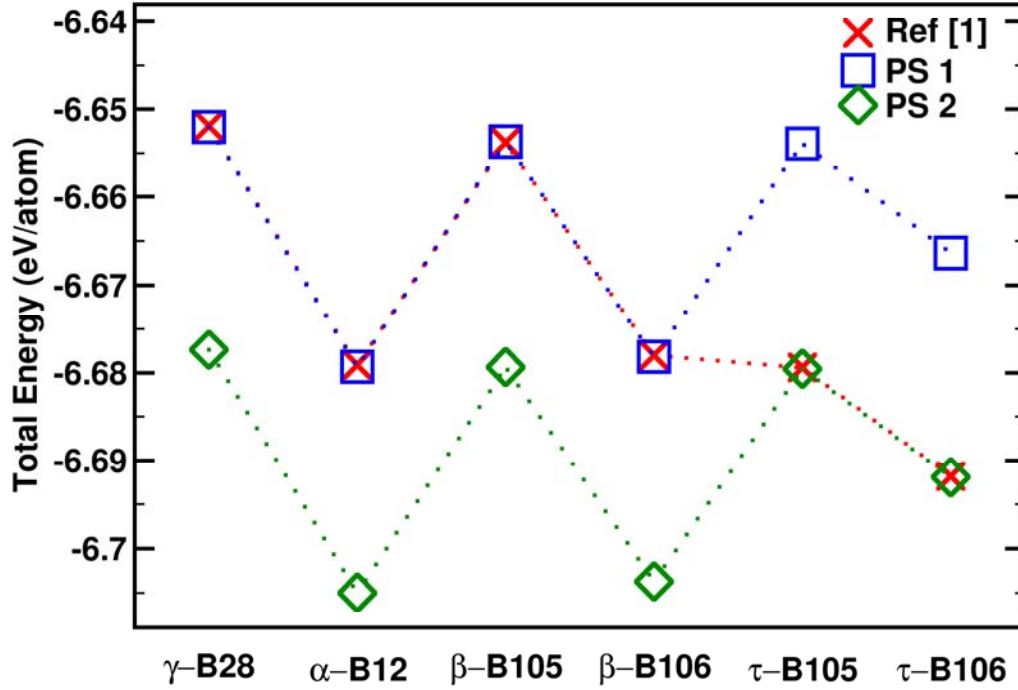[9] F. H. Horn, J. Appl. Phys. **30**, 1612 (1959).

Figures:

Figure 1: Total energies of boron allotropes calculated with two different pseudopotentials compared to the data published in ref [1]. It appears that the published data in ref [1] was generated with two different pseudopotentials: PS 1 for α-B12, β-B105, β-B106 and γ-B28, and PS 2 for τ-B105 and τ-B106.