Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information for

Semiconducting α'−boron sheet with high mobility and low all-boron contact resistance: A first-principles study

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I. GW0 results for α- and α′-boron sheet

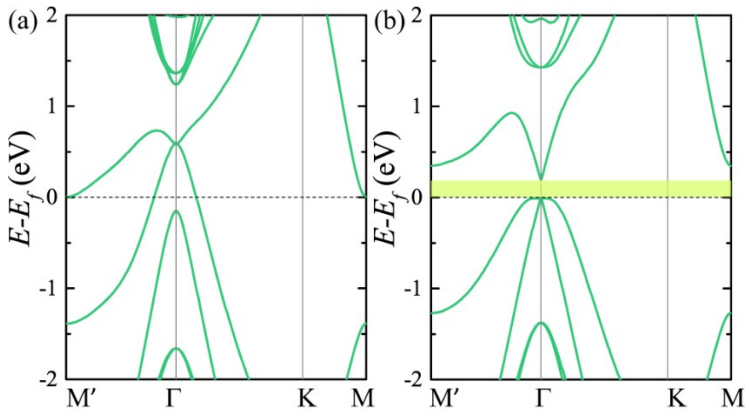

Figure S1. GW0 results for (a) α-boron sheet and (b) α′-boron sheet. Cyan donates the band gap in α′-boron sheet.

II. More TB model results for α- and α′-boron

The total Hamiltonian with nearest-neighbor, (8×8 matrix)

$$H=\begin{bmatrix} h_{11} & h_{12} & 0 & h_{14} & 0 & h_{16} & h_{17} & h_{18} \\ h_{21} & h_{22} & h_{23} & 0 & h_{25} & 0 & h_{27} & h_{28} \\ 0 & h_{32} & h_{33} & h_{34} & 0 & h_{36} & h_{37} & h_{38} \\ h_{41} & 0 & h_{43} & h_{44} & h_{45} & 0 & h_{47} & h_{48} \\ 0 & h_{52} & 0 & h_{54} & h_{55} & h_{56} & h_{57} & h_{58} \\ h_{61} & 0 & h_{63} & 0 & h_{65} & h_{66} & h_{67} & h_{68} \\ h_{71} & h_{72} & h_{73} & h_{74} & h_{75} & h_{76} & h_{77} & 0 \\ h_{81} & h_{82} & h_{83} & h_{84} & h_{85} & h_{86} & 0 & h_{88} \end{bmatrix}$$

note that some elements are zero, indicating they don't belong to nearest-neighbor. The selected lattice vector are $a_1 = a\begin{pmatrix}1 & 0\end{pmatrix}$, $a_2 = a(-\frac{1}{2} \quad \frac{\sqrt{3}}{2})$. For example, there are five nearest-neighbor atoms for B1 atom, which are B2, B4, B6, B7 and B8. The corresponding translation vectors from B1 to its nearest-neighbor boron are δ_{12}=-$a(\frac{\sqrt{3}}{2} \quad \frac{3}{2})$, δ_{14}=$a(1 \quad \frac{\sqrt{3}}{2})$, δ_{16}=$a(1 \quad 0)$, δ_{17}=$a(\frac{1}{2} \quad -\frac{\sqrt{3}}{2})$ and δ_{18}=$a(-1 \quad 0)$, where a is lattice constant of α-boron sheet. Thus, their Hamiltonian in reciprocal space can be read as following,

$$H_{12} = -\frac{t_1}{N}\sum_{\vec{k}} e^{-ia(\frac{\sqrt{3}}{2}k_x+\frac{3}{2}k_y)} C^{\dagger}_{\vec{k}_2} C_{\vec{k}_1},$$

$$H_{14} = -\frac{t_3}{N}\sum_{\vec{k}} e^{ia(k_x+\frac{\sqrt{3}}{2}k_y)} C^{\dagger}_{\vec{k}_4} C_{\vec{k}_1},$$

$$H_{16} = -\frac{t_3}{N}\sum_{\vec{k}} e^{iak_x} C^{\dagger}_{\vec{k}_6} C_{\vec{k}_1},$$

$$H_{17} = -\frac{t_2}{N}\sum_{\vec{k}} e^{ia(\frac{1}{2}k_x-\frac{\sqrt{3}}{2}k_y)} C^{\dagger}_{\vec{k}_7} C_{\vec{k}_1},$$

$$H_{18} = -\frac{t_2}{N}\sum_{\vec{k}} e^{-iak_x} C^{\dagger}_{\vec{k}_8} C_{\vec{k}_1}.$$

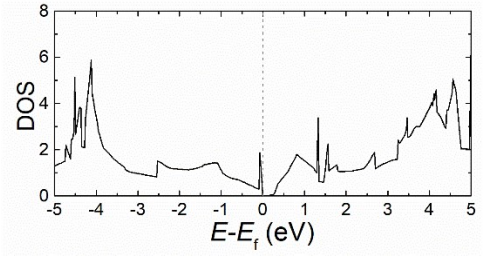

Figure S2. The DOS of semiconducting α' boron sheet using HSE06 functional.

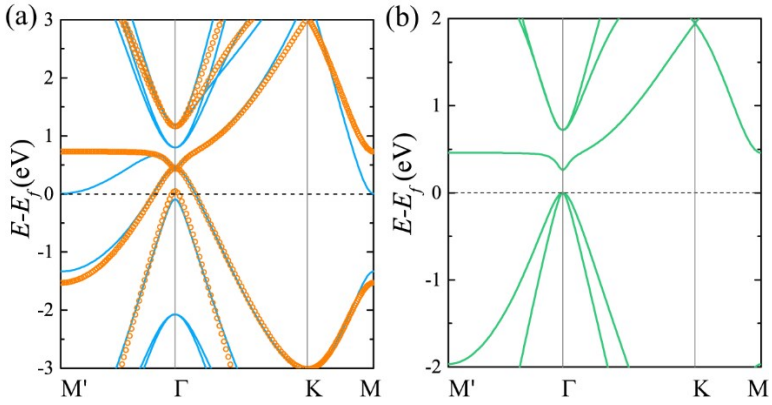

Figure S3. (a) TB model results for α-boron sheet. Blue lines are HSE06 results. Orange circles donate TB model fitting results. (b) TB model results for α′-boron sheet with t_2=1.4 eV, ε_2=-2.0 eV.

III. More carrier mobility results for α′- and β^S_3 boron sheet

Based on Boltzmann transport equations, the anisotropic electrical conductivity $\boldsymbol{\sigma}$ is expressed as following,

$$\sigma_{ij}(\mu,T)=\frac{e^2}{V}\int_{-\infty}^{+\infty}d\varepsilon\sum_{n,k}\left(-\frac{\partial f(\varepsilon,\mu,T)}{\partial\varepsilon}\right)v_i(n,k)v_j(n,k)\tau(n,k)\delta(\varepsilon-E_{n,k}),$$

where $f(\varepsilon,\mu,T)$ is the usual Fermi-Dirac distribution function, defined as

$$f(\varepsilon,\mu,T)=\frac{1}{e^{(\varepsilon-\mu)/K_BT}+1}$$

$E_{n,k}$ is the energy of the n−th band at k, $v_i(n, k)$ is the i−th component of the band velocity at (n, k), and τ is electron relaxation time. In addition, detailed description of the calculations of electrical conductivity can be found in *PRB*, 68, 125210 (2003) and *Comput. Phys. Commun.* 2008, 178, 685–699. In this work, we fitted τ from the calculated hole mobility of α′-boron sheet with Eq. (4) in main text, which is about 90 fs (Figure S3).

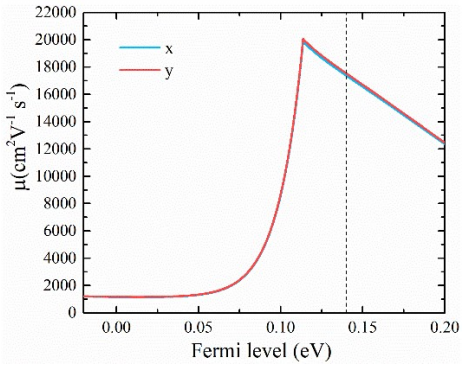

Figure S4. Carrier mobility for α′-boron sheet using $\mu=\sigma/ne$ along Γ-M′ (x) and Γ-K (y). Note that the electron mobility is inaccurate, which is caused by the small band gap in α′-boron sheet.

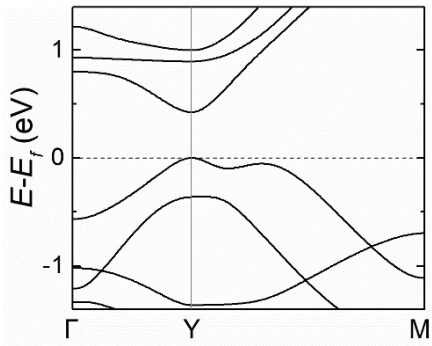

Figure S5. The band structure of semiconducting β_3^S boron sheet using HSE06 functional.

IV. The structures of selected metallic boron sheet

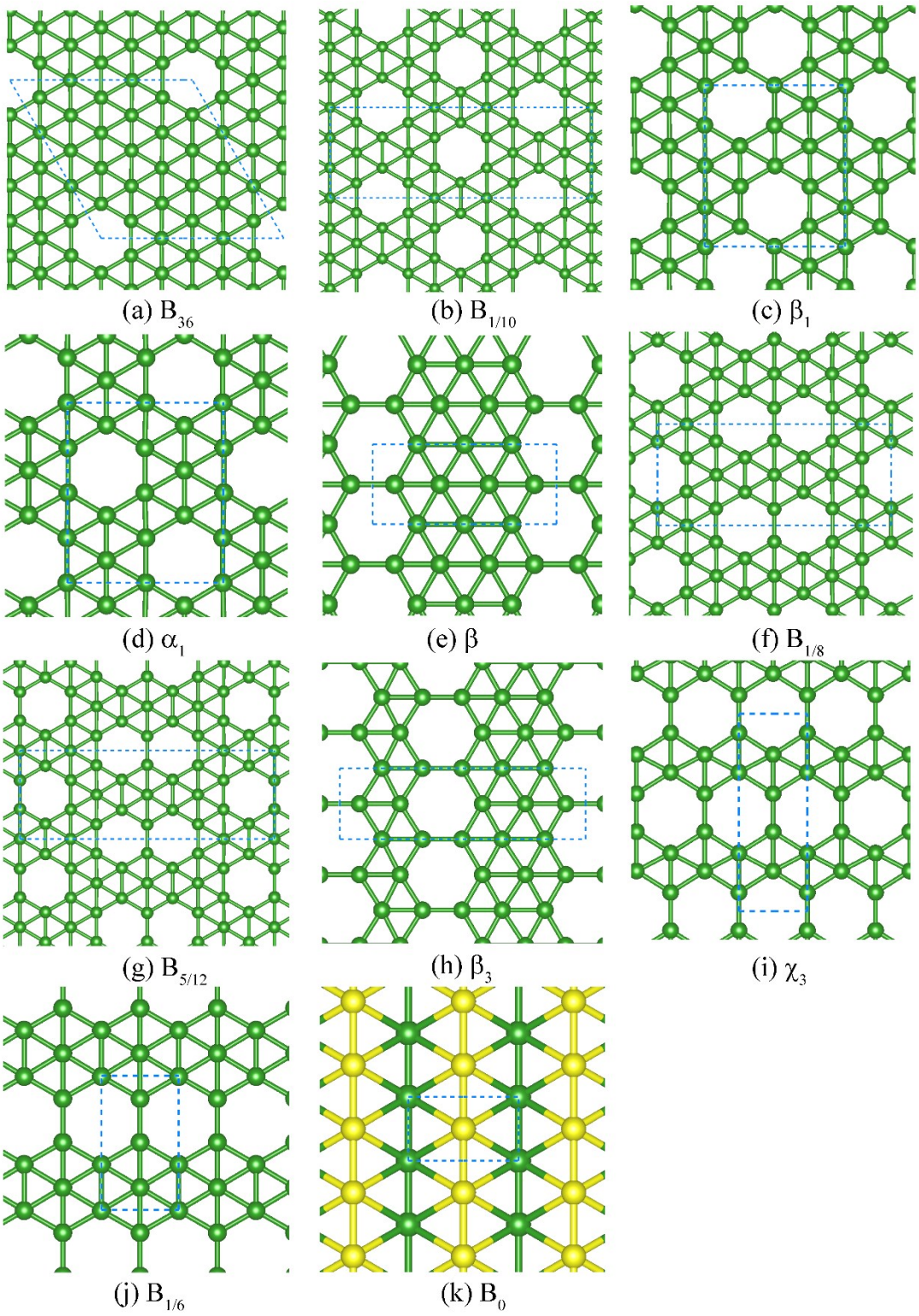

Figure S6. Selected stable metallic boron sheet for Schottky barrier calculations. Blue frames donate the selected unit cell. Yellow atoms indicate boron atoms moving outward/inward from the plane.