Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Spindle Nodal Chain in Three-Dimensional α' Boron

Yan Gao[1], Yuee Xie[1], Yuanping Chen[1]*, Jinxing Gu[2], and Zhongfang Chen[2]

[1]*School of Physics and Optoelectronics, Xiangtan University, Xiangtan, 411105, Hunan, China*

[2]*Department of Chemistry, University of Puerto Rico, Rio Piedras Campus, San Juan, Puerto Rico 00931, United States*

Corresponding author: chenyp@xtu.edu.cn

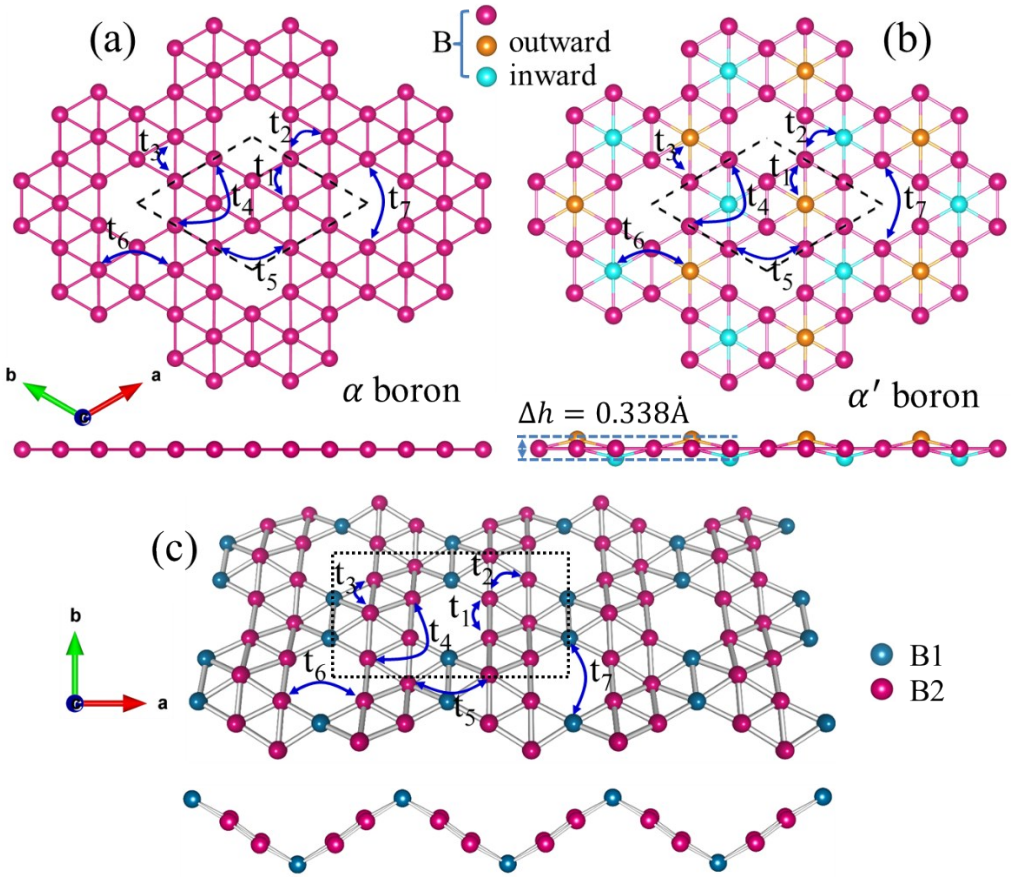

Figure S1. Top and side views of (a) α boron sheet and (b) α' boron sheet, and (c) bare single-layer wiggle α' sheet. In α' sheet, the atoms in the hexagonal centers are slightly inward (azury atoms) or outward (yellow atoms) the plane about 0.169 Å. The primitive cells of the three structures are shown in the dotted boxes. The symbols $t_1 \sim t_7$ represent hopping energies between atoms. The structural parameters of the three structures can be seen in Table 1.

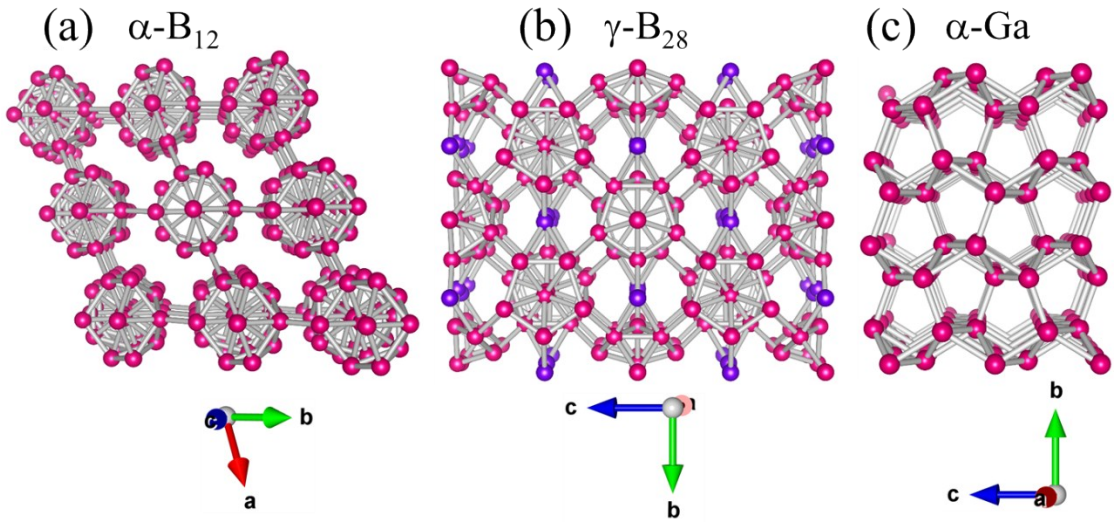

Figure S2. The optimized atomic structure of (a) α-B_{12}, (b) γ-B_{28}, and (c) α-Ga. For the γ-B_{28} structure, two oppositely charged sublattices are marked by different colours (anionic, red; cationic, purple). The structural parameters of the three structures can be seen in Table 1.

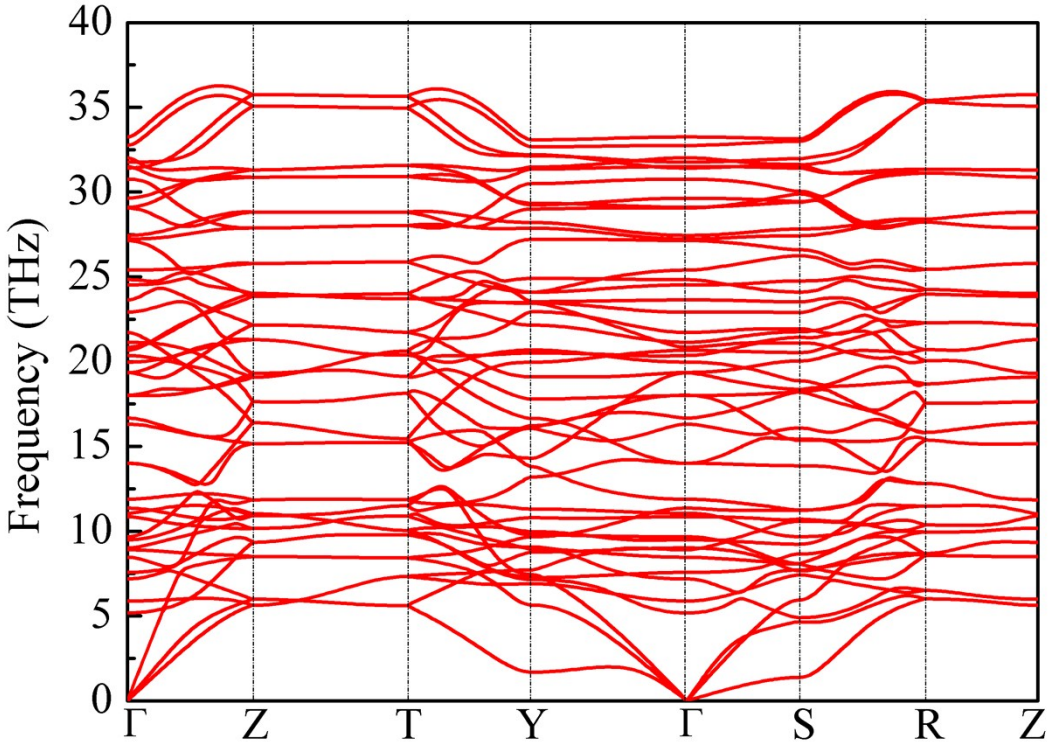

Figure S3. Phonon dispersion of the 3D-α' boron. It reveals the absence of any imaginary frequencies over the entire BZ, suggesting that the structure is dynamically stable.

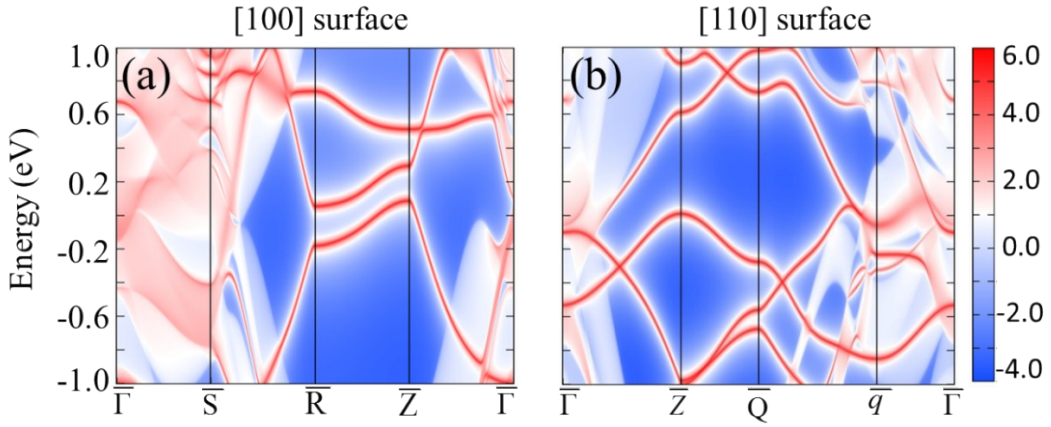

Figure S4. Surface states of 3D-α' boron on the surfaces [100] (a) and [110] (b).

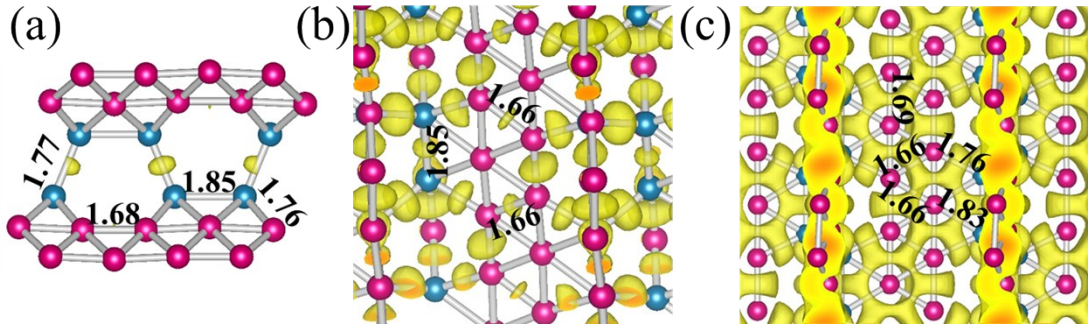

Figure S5. The electronic localization function (ELF) data of 3D-α' boron with the isosurface value as (a) 0.90, (b) 0.80, and (c) 0.70. Some typical bond lengths are recorded near the corresponding bonds for further discussion.

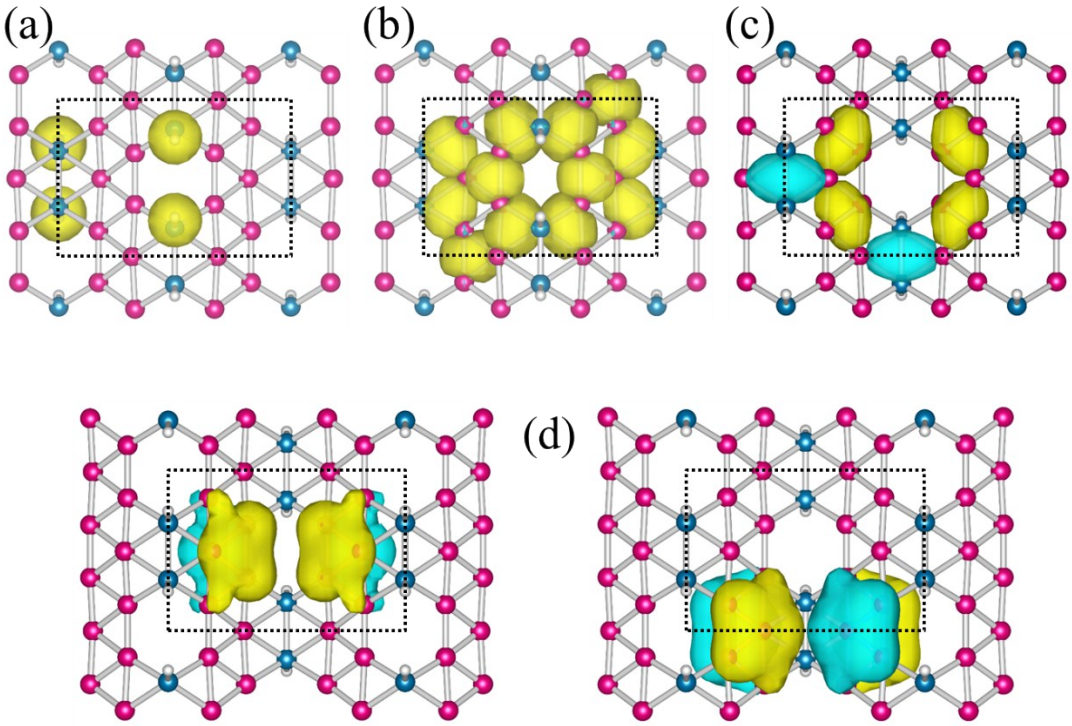

Figure S6. The SSAdNDP chemical bonding analysis of 2D BH-sheet. Totally 26 bonds are exhibited, including (a) four 2c-2e σ bonds, ONs = 1.91 |*e*|, (b) twelve 3c-2e σ bonds, ONs = 1.94 |*e*|, (c) six 4c-2e σ bonds, ONs = 1.74 |*e*|, and (d) four 5c-2e π bonds, ONs = 1.88/1.64 |*e*|.

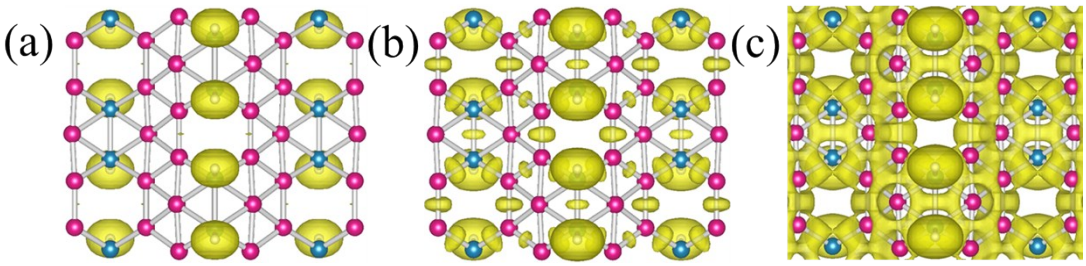

Figure S7. The electronic localization function (ELF) data of 2D-BH sheet with the isosurface value as (a) 0.90, (b) 0.80, and (c) 0.70. Clearly shows the B-H single bond, 3c-2e σ bond, 4c-2e σ bond and 5c-2e π bond.

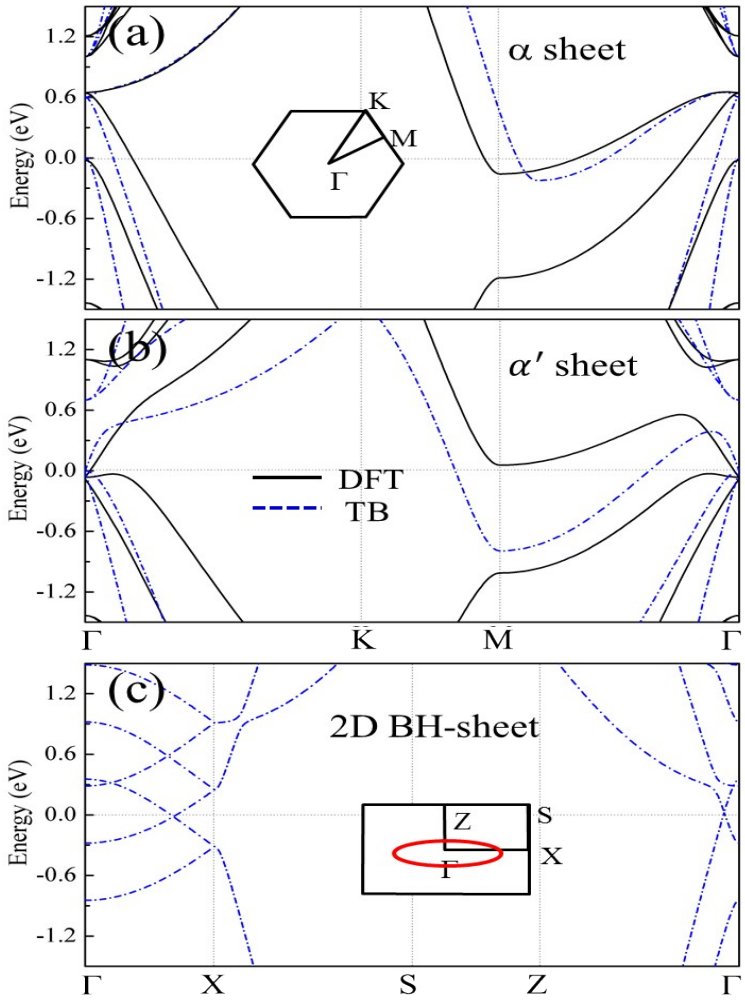

Figure S8. (a) Tight-binding band structures of α boron sheet with parameters are t_1=-2.8, t_2=-2.8, t_3=-2.8, t_4=-0.7, t_5=-0.3, t_6=-0.2, t_7=-0.2 and onside energy e=-0.9. Inset: the first BZ showing the high-symmetry k points. (b) Tight-binding band structures of α' boron sheet with parameters t_1=-2.8, t_2=-2.8, t_3=-2.8, t_4=-0.7, t_5=-0.46, t_6=-0.35, t_7=-3.5 and onside energy e=-1.4. (c) Tight-binding band structures of 2D BH boron sheet with parameters t_1=-2.4, t_2=-2.8, t_3=-2.8, t_4=-0.16, t_5=-0.5, t_6=-0.7 and onside energy e=0.0. Inset: the first BZ showing the high-symmetry k points and red nodal ring. All the values are in unit of eV. For comparison, the DFT results for α and α' boron sheets are shown in (a-b) with solid lines, respectively.

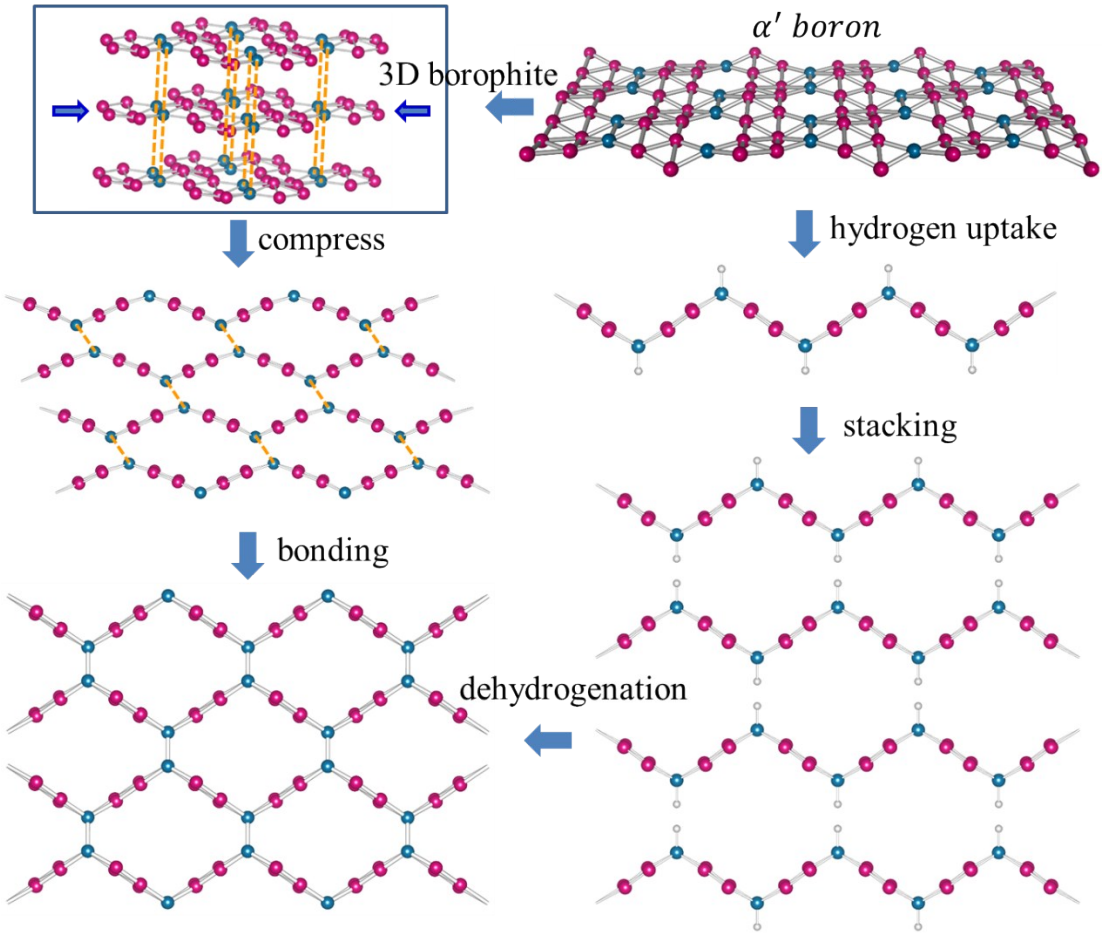

Figure S9. Two possible routes to fabricate the 3D-α' boron, based on the unit of α' boron sheets: (1) Compressing the α' boron sheets: in this approach, the α' boron sheets are first stacked to a 3D layered structure, then a compressive strain is applied on the plane of boron sheets. The strong interactions between wiggle sheets could form linkages between layers and thus result in the bulk. Note that this method has been used to prepare the 3D carbon networks from graphene. (2) Dehydrogenation of the stacked 2D BH-sheets: in this process, the 2D BH-sheets are stacked, and the dehydrogenation reaction leads to the formation of 3D-α' boron.

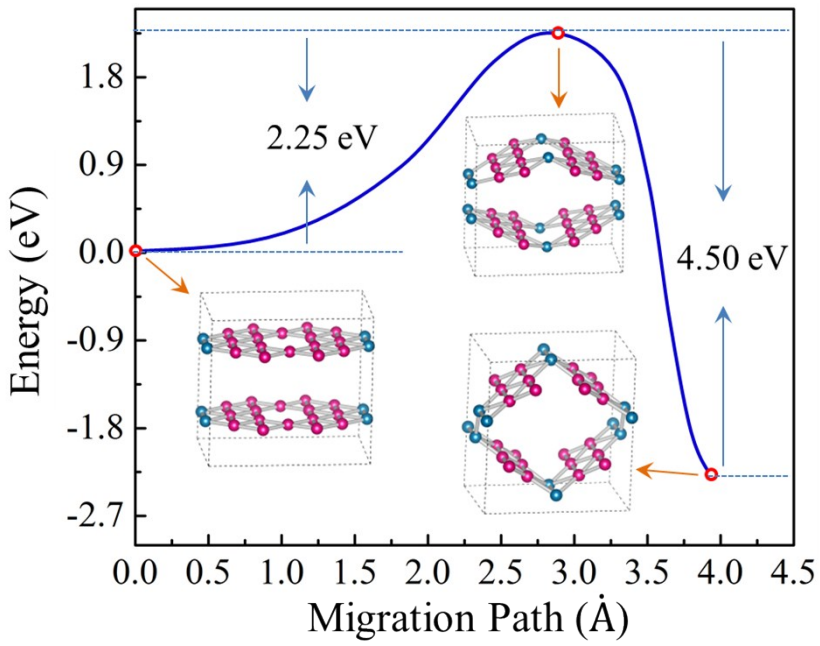

Figure S10. Evaluation for the phase transition barrier form 3D α' boron sheets to 3D-α' boron. It is evaluated by using the climbing image nudged elastic band (Cl-NEB) technique.