Global Minima Search for Sodium and Magnesium Adsorbed Polymorphic Borophene

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Supporting Information

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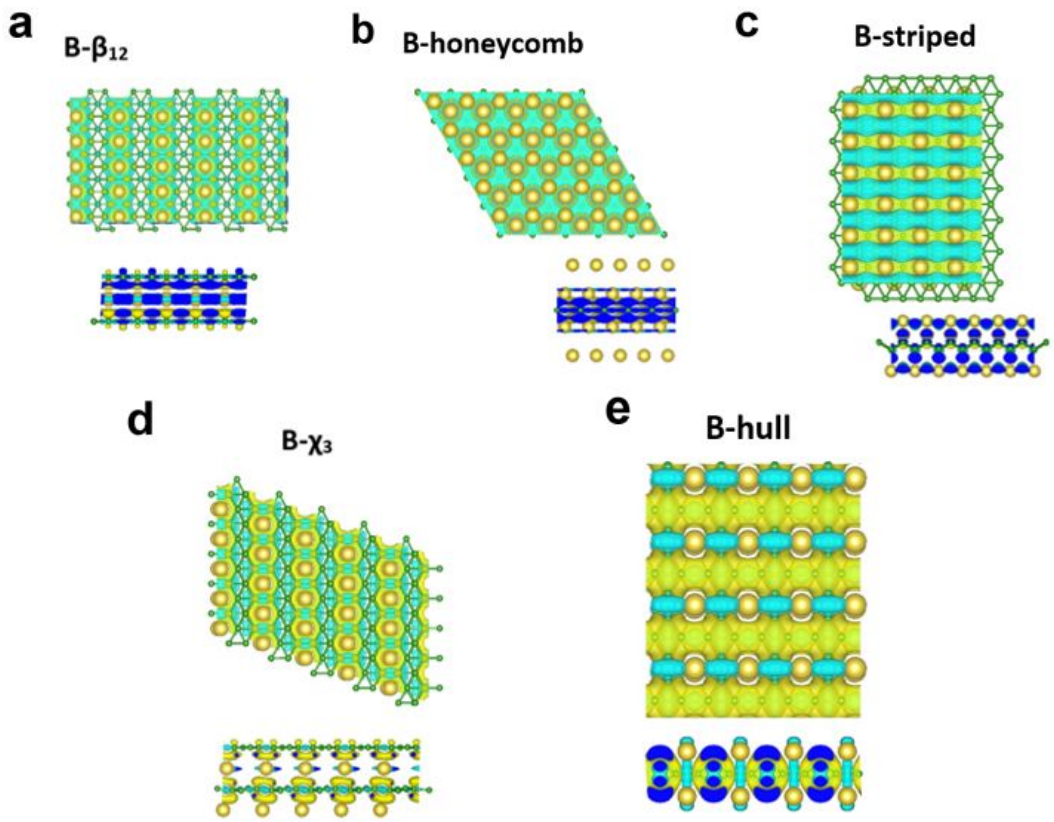

Figure S1. Top and side views of structures showing charge density difference for most stable Na-adsorbed borophene phases found in bottom-up evolutionary structure searching approach. The β_{12}, honeycomb, striped and χ_3 phases are shown in parts (a), (b), (c) and (d), respectively. Striped and honeycomb phases are manually constructed. The structure in part € is a new structure obtained from the convex hull at composition ratio of 0.25. The green and yellow balls represent B and Na atoms respectively. The blue regions represent the electron depletion and yellow regions represent electron accumulation.

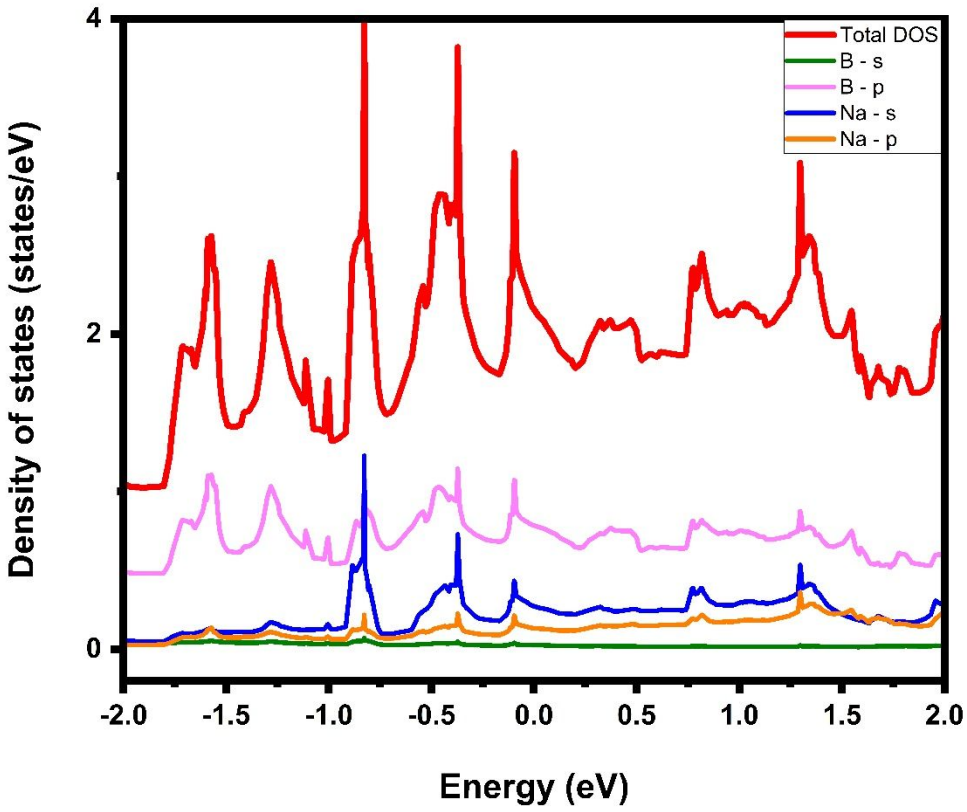

Figure S2: Total Density of states (DOS) and Projected DOS for s and p orbitals of boron and sodium atoms for the most stable Na-adsorbed χ_3 borophene phase obtained through bottom-up structure searching approach. Density of states for s and p orbitals of sodium are magnified by 5 times.

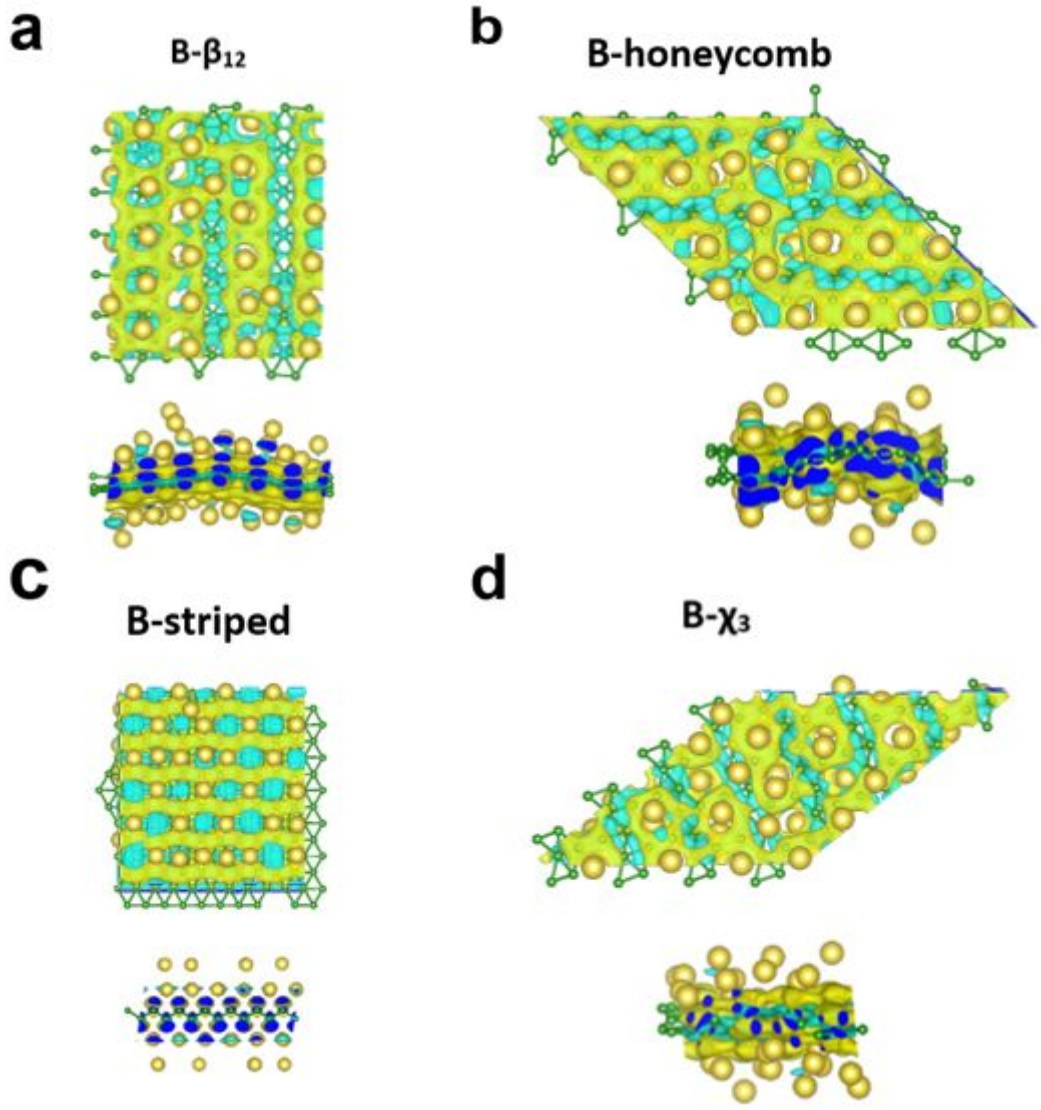

Figure S3. Top and side views of structures showing charge density difference for most stable Na-adsorbed borophene phases found in top-down AIRSS approach for β_{12}, honeycomb, striped and χ_3 phases are shown in parts (a), (b), (c) and (d), respectively. The green and yellow balls represent B and Na atoms respectively. The blue regions represent the electron depletion and yellow regions represent electron accumulation.

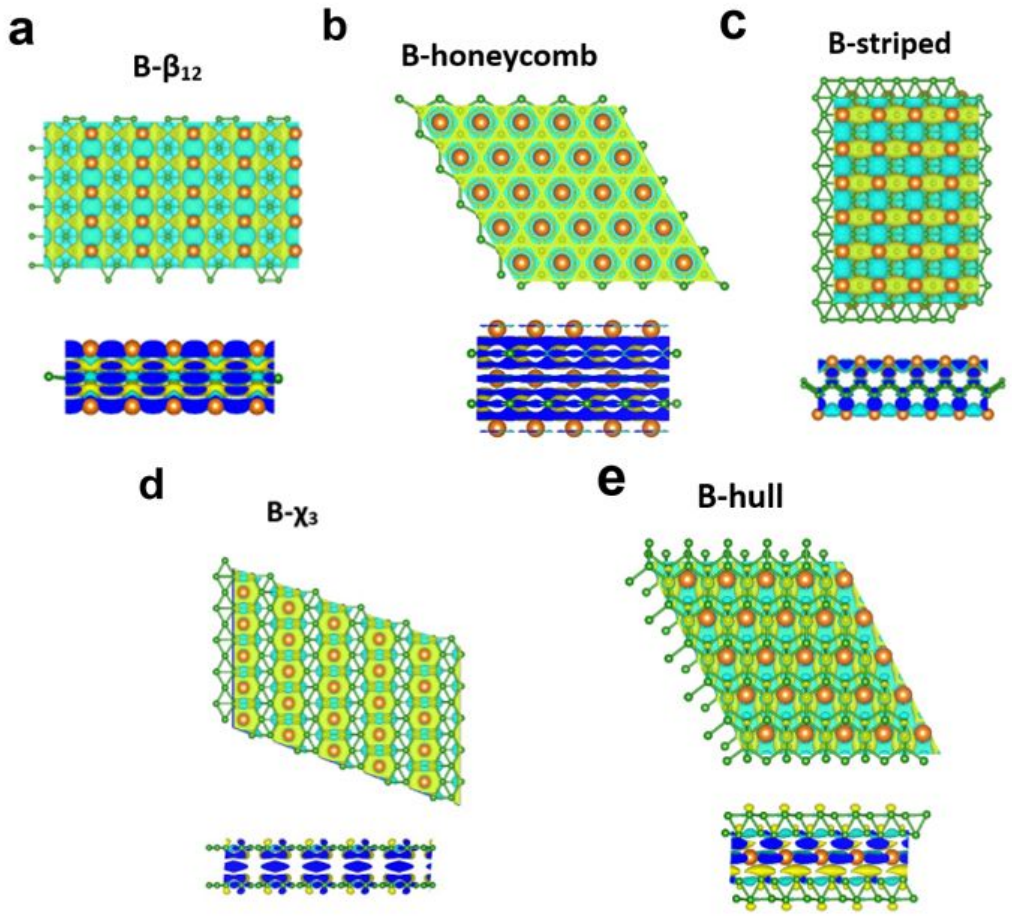

Figure S4. Top and side views of structures showing charge density difference for most stable Mg-adsorbed borophene phases found in bottom-up evolutionary structure searching approach for β_{12}, honeycomb, striped and χ_3 phases are shown in parts (a), (b), (c) and (d), respectively. Striped and honeycomb phases are manually constructed. The structure in part (e) is new structure obtained from the convex hull at composition ratio of 0.11. The green and orange balls represent B and Mg atoms respectively. The blue regions represent the electron depletion and yellow regions represent electron accumulation.

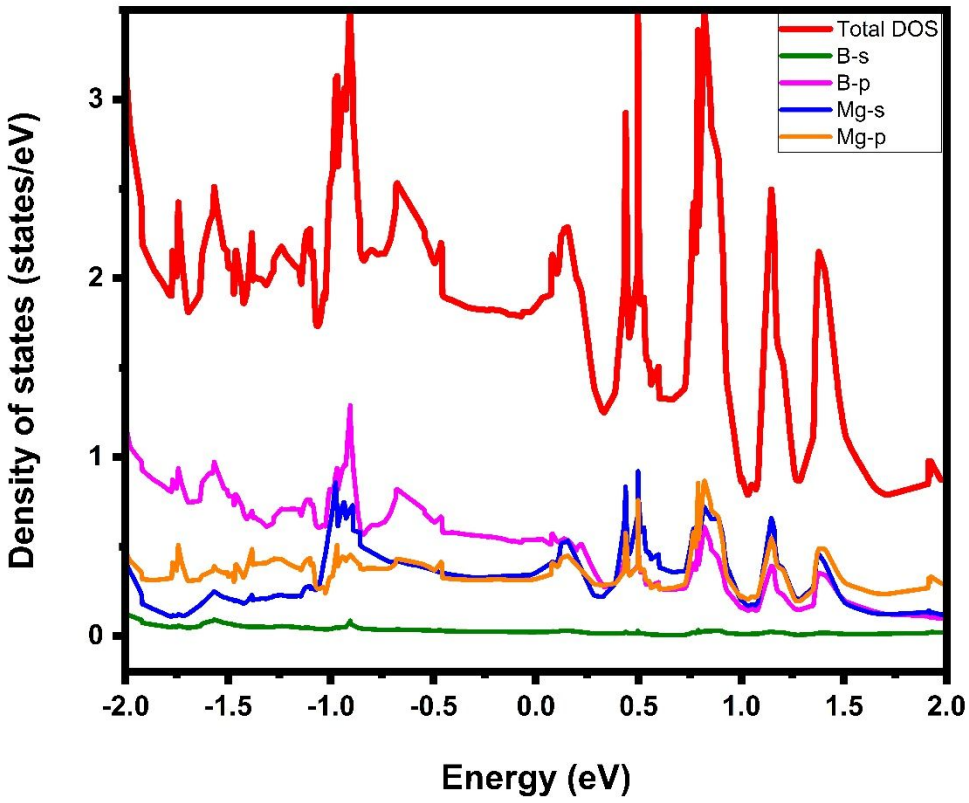

Figure S5: Total Density of states (DOS) and Projected DOS for s and p orbitals of boron and magnesium atoms for the most stable Mg-adsorbed bilayer honeycomb borophene phase obtained through bottom-up structure searching approach. Density of states for s and p orbitals of magnesium are magnified by 5 times.

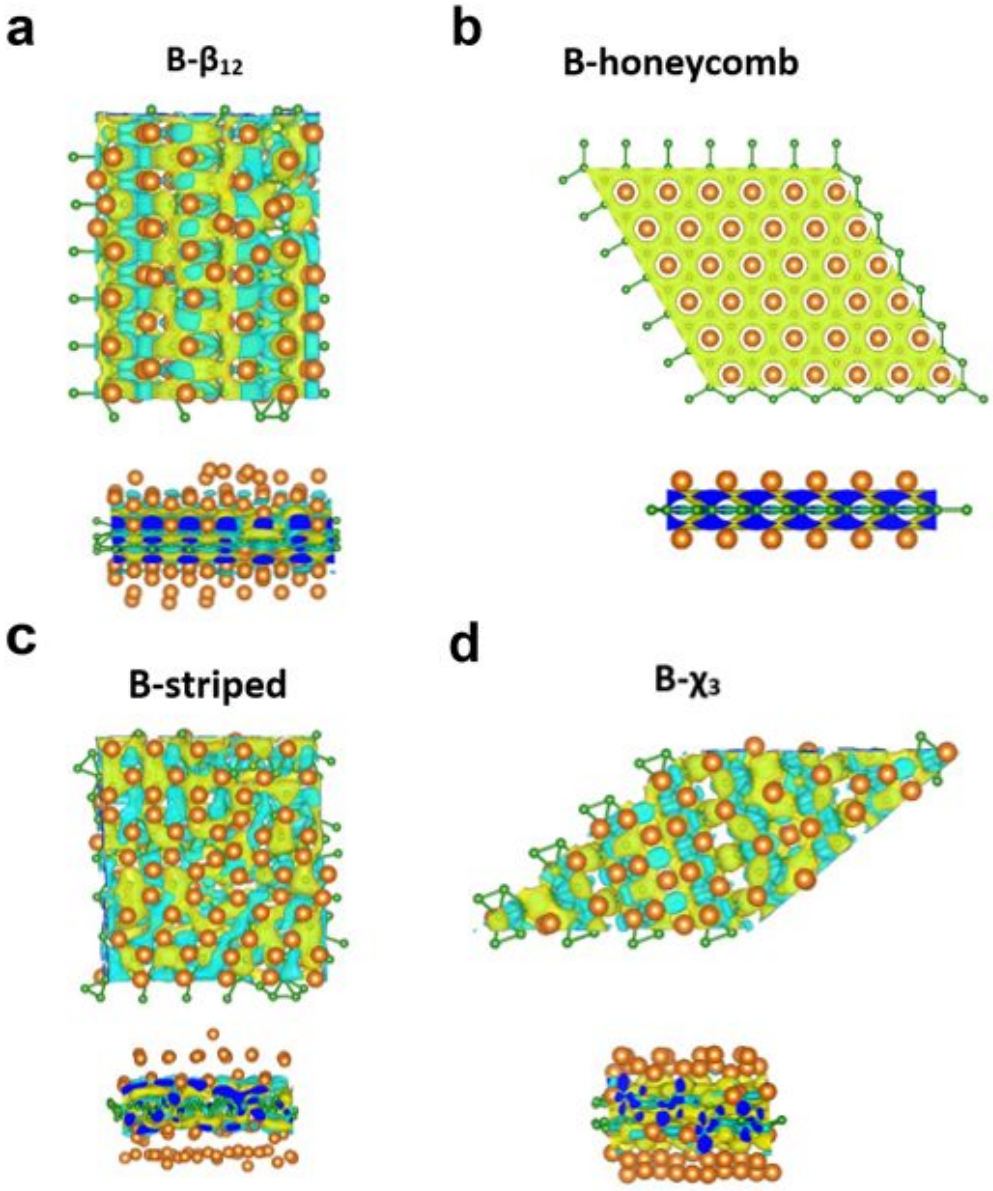

Figure S6. Top and side views of structures showing charge density difference for most stable Mg-adsorbed borophene phases found in top-down AIRSS approach for β_{12}, honeycomb, striped and χ_3 phases are shown in parts (a), (b), (c) and (d), respectively. The green and orange balls represent B and Mg atoms respectively. The blue regions represent the electron depletion and yellow regions represent electron accumulation.

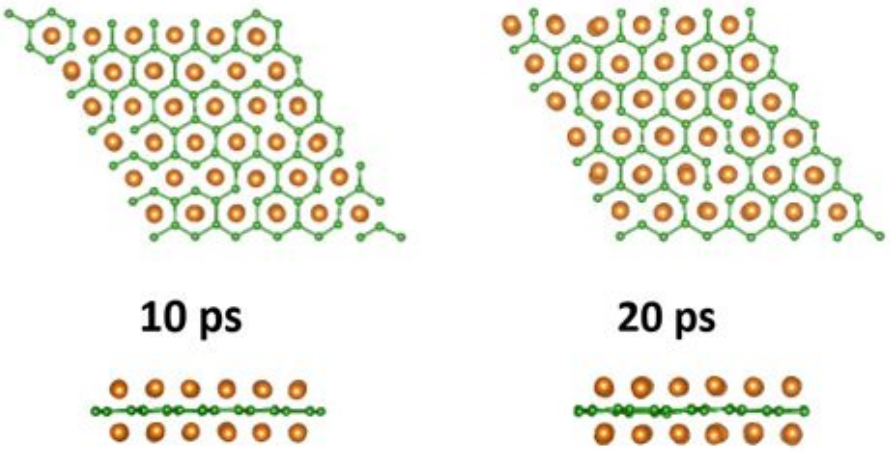

Figure S7: Top and side-view of AIMD snapshots of AIRSS-found most stable phase for Mg-adsorbed borophene. The green and orange balls represent B and Mg atoms respectively. At 10ps, the 10K-300 K heating of the structure finishes, and then it is subjected to 300 K temperature up to 20 ps.