Supporting Information: Calcium atom modified boron phosphide (BP) biphenylene as an efficient hydrogen storage material

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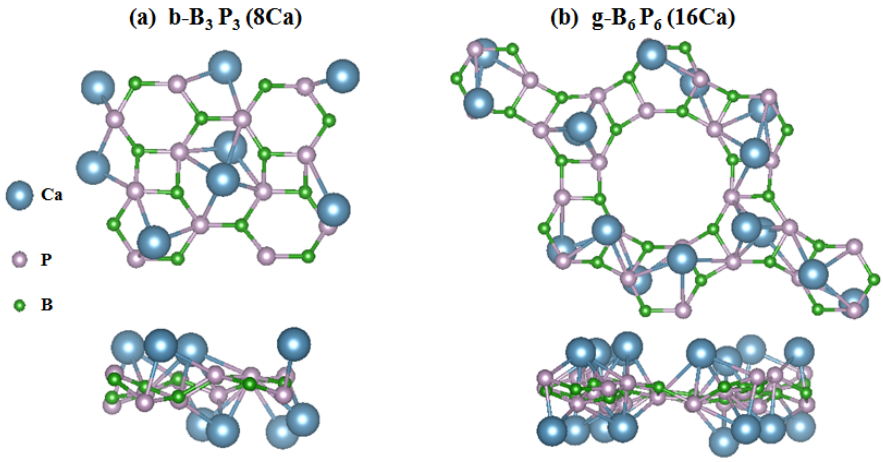

Figure 1: Relaxed structures of (a) $b - B_3P_3(Ca)$ and (b) $g - B_6P_6(Ca)$ structures.

To provide a hint on the bonding nature of $b - B_3P_3(8Ca)$ and $g - B_6P_6(16Ca)$ structures, the total density of states (TDOS) and projected density of states (PDOS) are plotted in Fig. S2. It is evident from the plots that an interesting change in the PDOS occurs, with the emergence of new states at the Fermi level due to the overlapping of the electronic states of the Ca atoms with those of the BP surface.

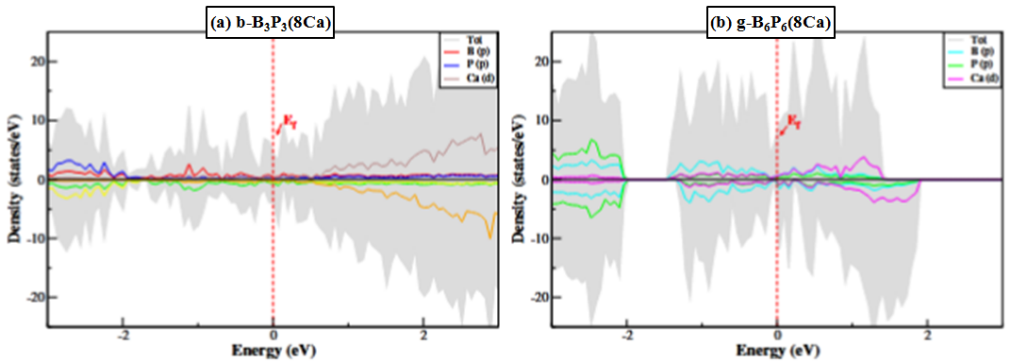

Figure 2: Total (TDOS) and Projected (PDOS) Density of States of (a) $b - B_3P_3(Ca)$ and (b) $g - B_6P_6(Ca)$ structures: Highlighting B (p), P (p), and Ca (d) Contributions

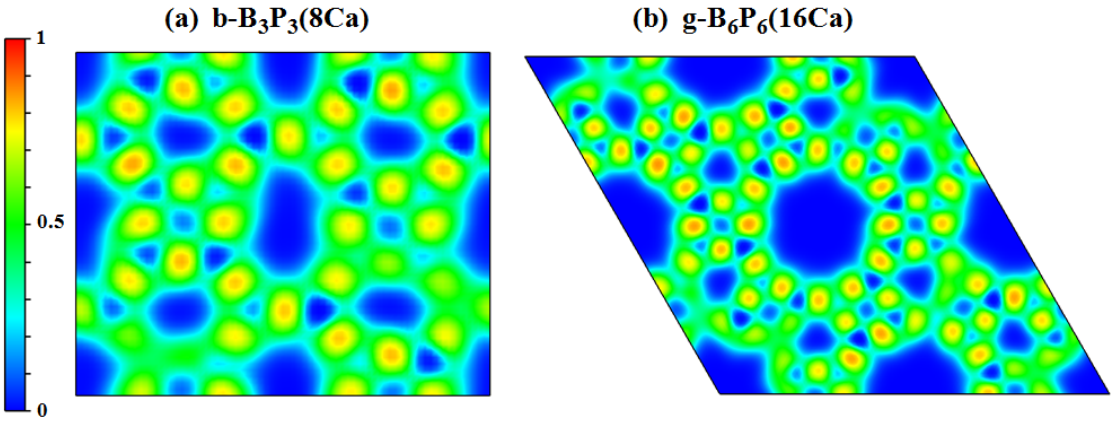

Figure 3: Electron Localization Function (ELF) of (a) $b - B_3P_3(8Ca)$ and (b) $g - B_3P_3(16Ca)$ structures.

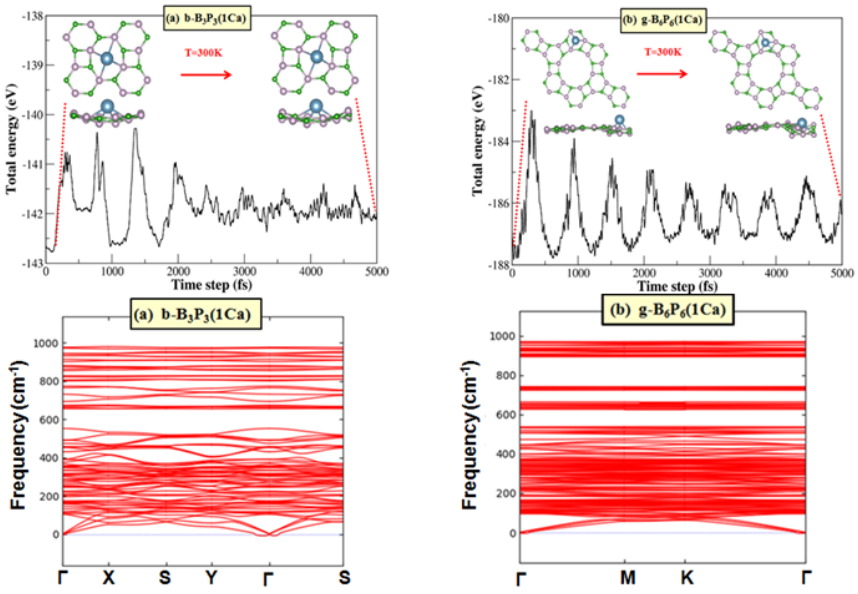

Figure 4: Molecular dynamics simulation of (a) $b - B_3P_3(8Ca)$ and $g - B_3P_3(16Ca)$ structures at T=300K

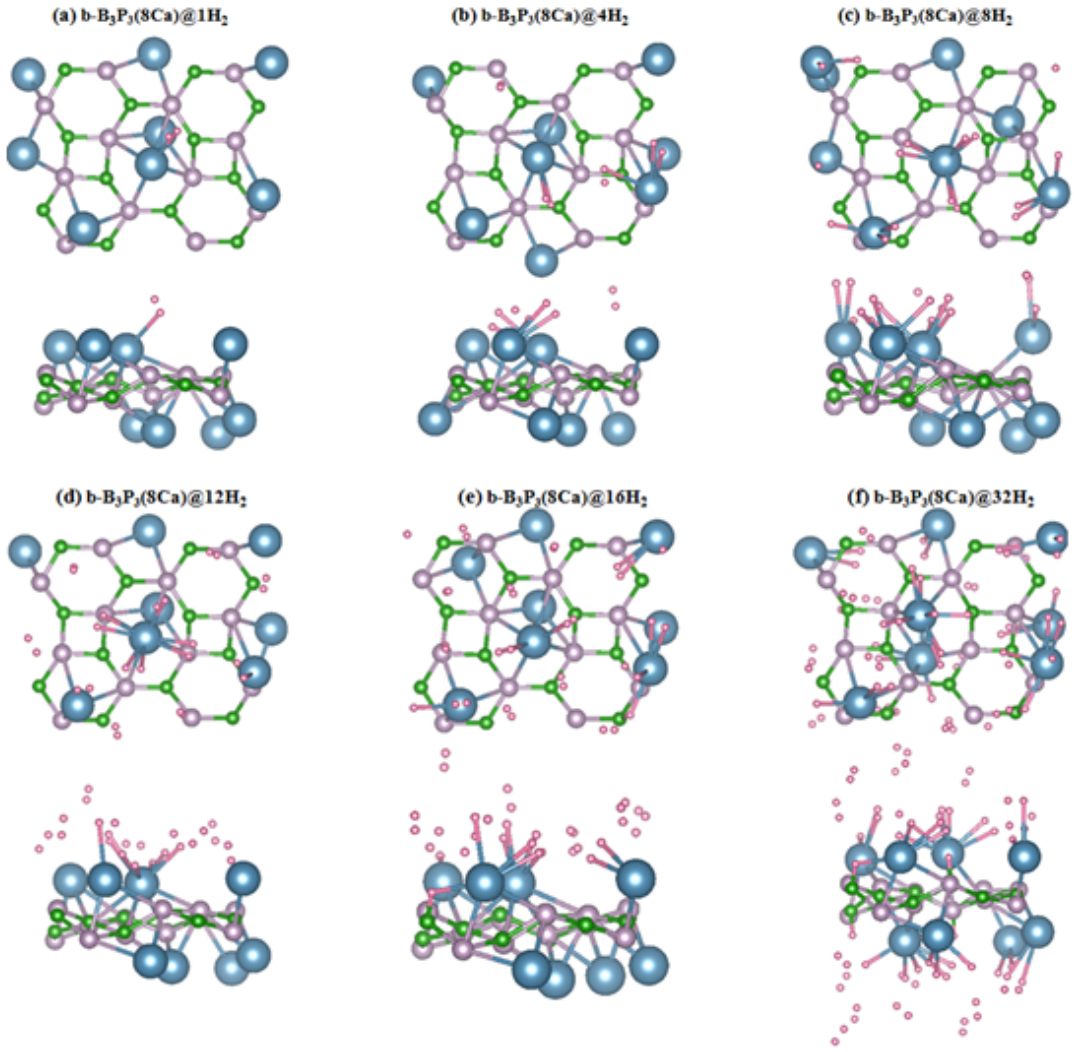

Figure 5: Optimized structures of several H_2 molecules ($1H_2$,$4H_2$, $8H_2$, $12H_2$, $16H_2$, $32H_2$) on $b - B_3P_3(8Ca)$ structure: Top and side views

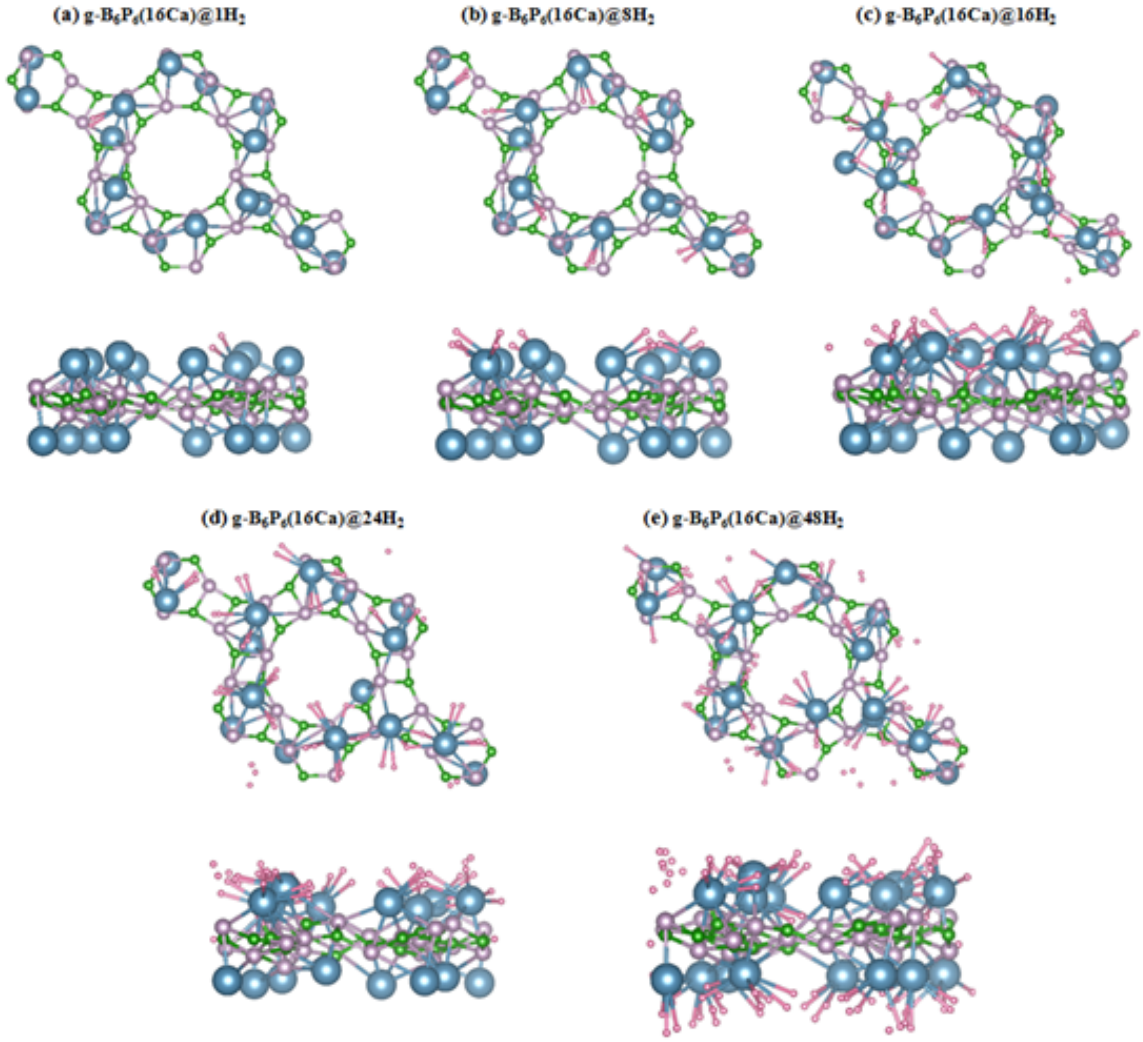

Figure 6: Optimized structures of several H_2 molecules ($1H_2$, $8H_2$, $16H_2$, $24H_2$, $48H_2$) on $g - B_6P_6(8Ca)$ structure: Top and side views

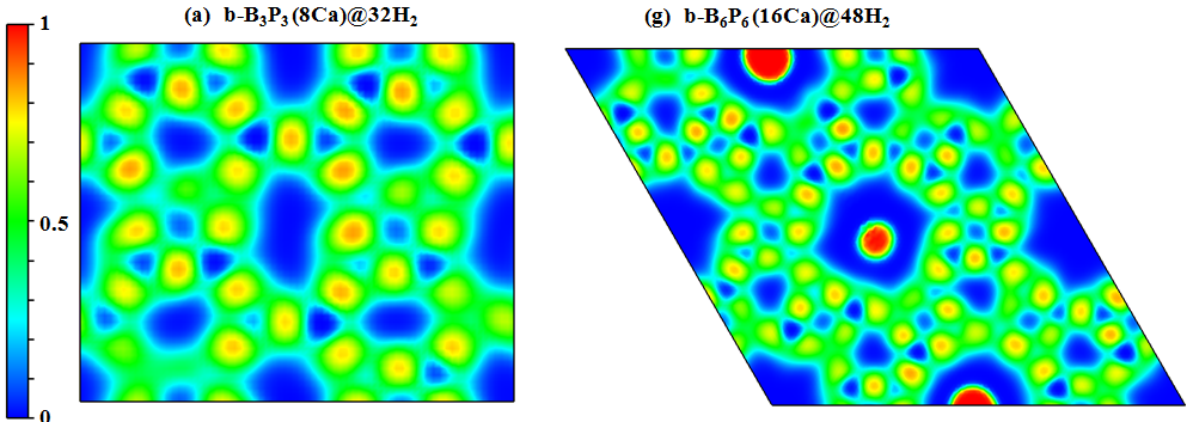

Figure 7: Electron Localization Function (ELF) of (a) $b - B_3P_3(8Ca)@32H_2$ and (b) $g - B_3P_3(8Ca)@48H_2$ structure.

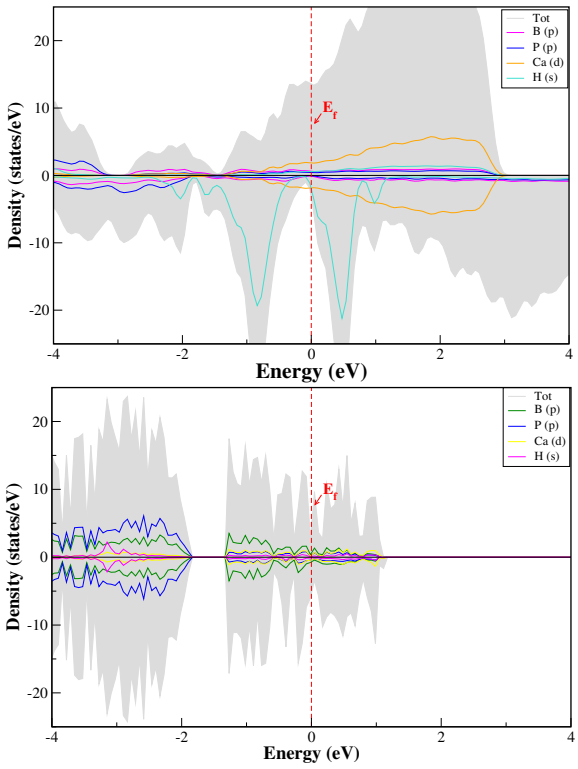

Figure 8: Total (TDOS) and Projected (PDOS) Density of States of (a) $b - B_3P_3(8Ca)@32H_2$ and (b) $g - B_6P_6(16Ca)@48H_2$ structures: Highlighting B (p), P (p), and Ca (d) and H (s) Contributions