

## Electronic supplementary information (ESI)

# Hydrogen storage characteristics of Li and Na decorated 2D Boron Phosphide

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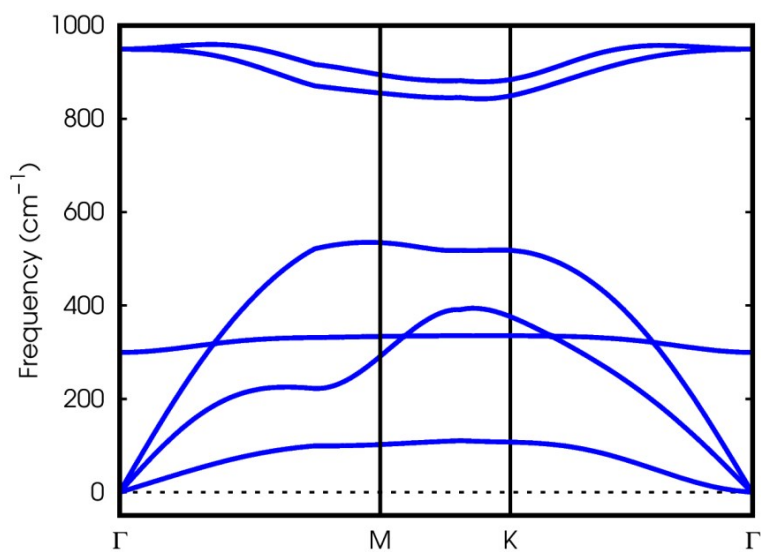
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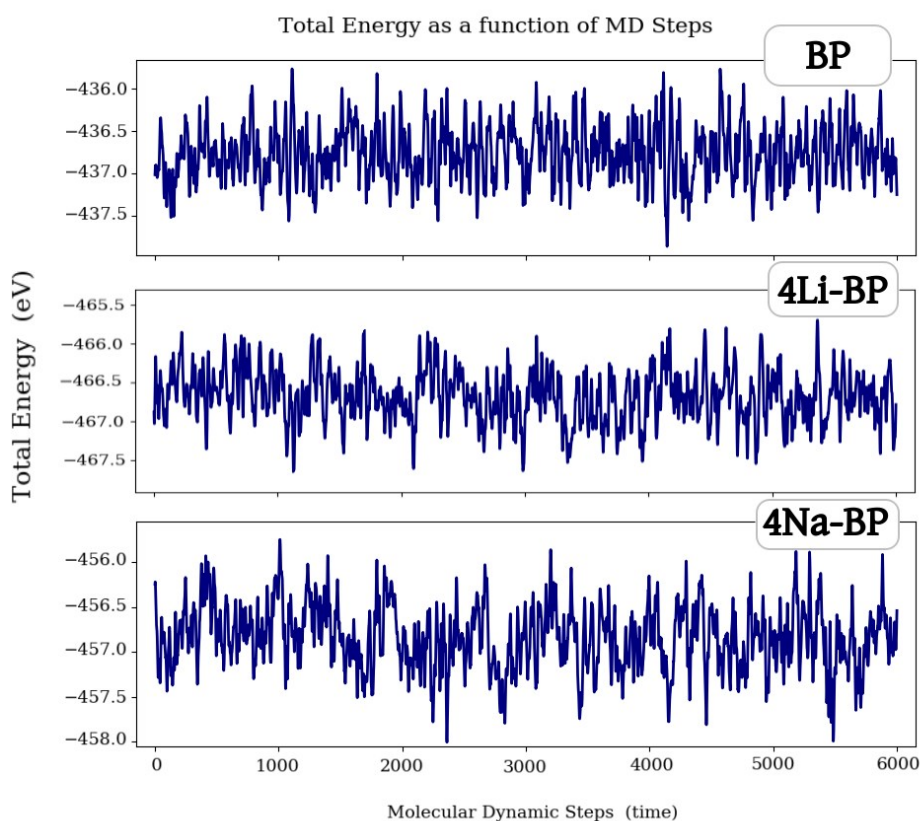
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**Figure S1.** Dynamical stability of 2D BP monolayer, the phonon dispersion pattern along the k-vectors with high symmetry.



**Figure S2.** Thermal stability of 2D BP, 4Li@BP and 4Na@BP monolayers, the variation of the total-energy between 0 and 6 ps during the ab-initio molecular dynamics (AIMD) simulations at room temperature.