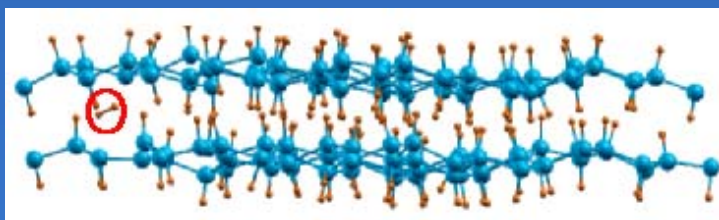
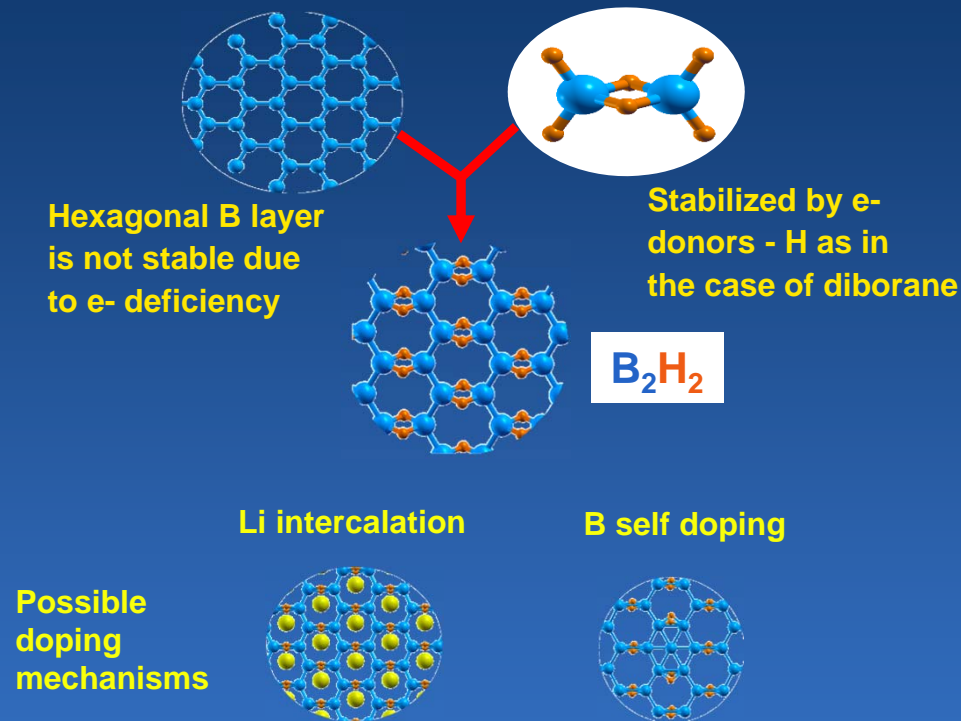


# Charging-assisted hydrogen release mechanism in layered boron hydride

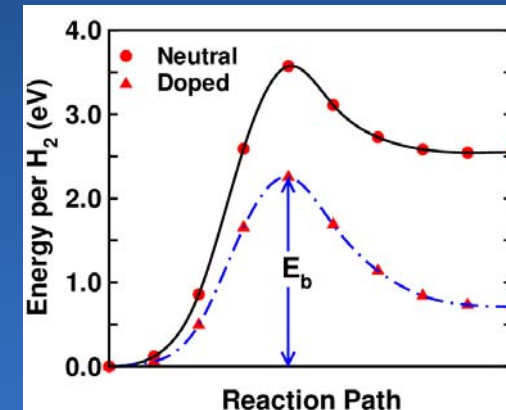
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MD simulations showing the stability of the structure and the release of hydrogen molecules

A novel layered solid boron hydride structure ( $B_2H_2$ ) consisting of hexagonal boron network and bridge hydrogen which has a gravimetric capacity of 8 wt% hydrogen is predicted.

We further investigate a charging-assisted hydrogen release mechanism, using both nudged elastic band method and ab initio molecular dynamics simulations.



NEB calculations show reduced hydrogen release energy barrier upon charge doping

## Publications

1. Tesfaye A. Abteu and Peihong Zhang, Phys. Rev. B 84, 094303 (2011)
2. Tesfaye A. Abteu, Bi-ching Shih, Pratibha Dev, Vincent H. Crespi, and Peihong Zhang, Phys. Rev. B 83, 094108 (2011)