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

Possible doping mechanisms
- Li intercalation
- B self doping

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

Publications