Light Metal Mediated Hydrogen Storage Capacity of Graphene Nanoribbons

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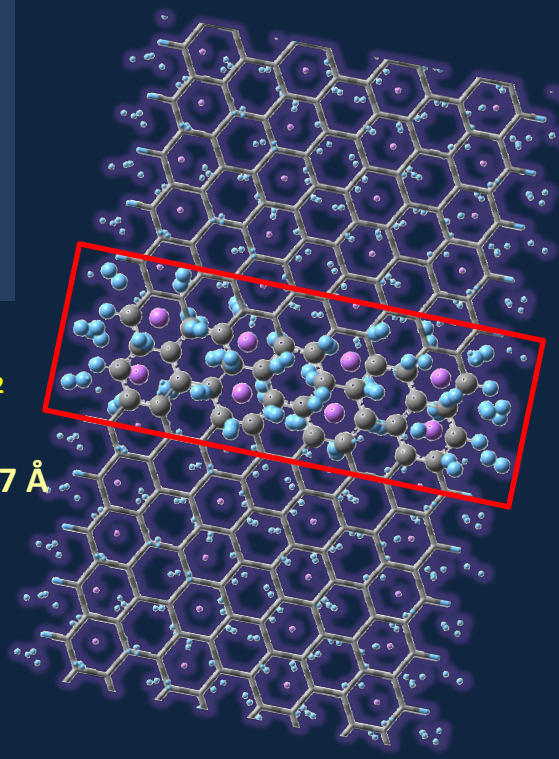
Using first principles methods, we study light metal absorption on the surface of low-dimensional graphenes, including graphene nanoribbons and porous graphenes. We try to optimize the structures to attain the higher charge transfer possible between the metal adsorbant and substrate. This optimization will lead to a stronger interaction between H molecules and metal ions.

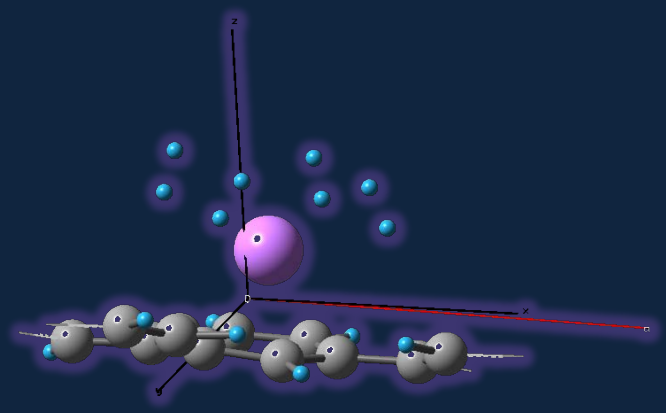


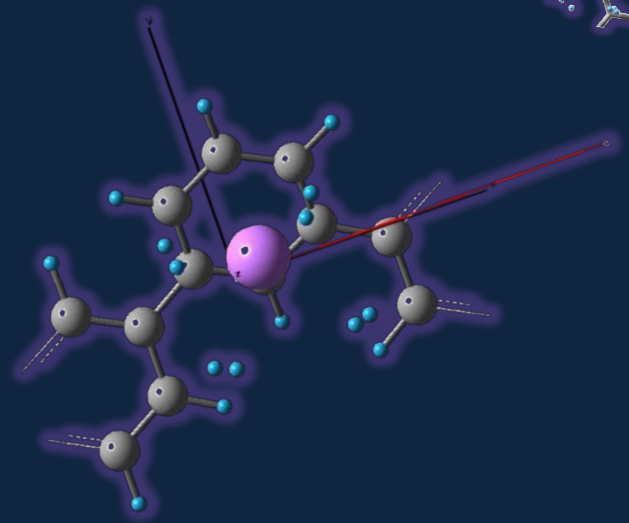
Zigzag nanoribbons + Li + $4H_2$

Eb(eV/1H_2) = 0.241 eV
Li-H distance = 2.026 and 2.847 Å
H-H bond = 0.778 Å

Low-dimensional porous graphene + Li + $4H_2$

Eb (eV/1H_2) = 0.237 eV
Li-H distance = 2.260 Å
H-H bond = 0.775 Å





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