Intercalation of boron nitride quantum dots with Lithium: boron nitride as a protecting layer for a Lithium-ion battery and a spin-dependent photon emission device

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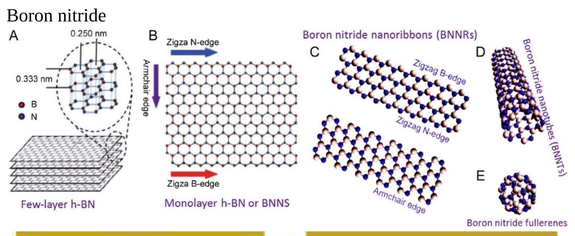
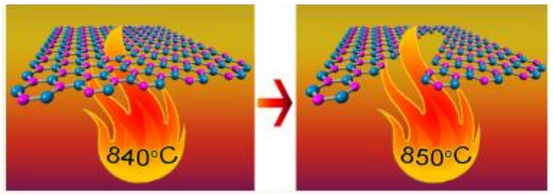
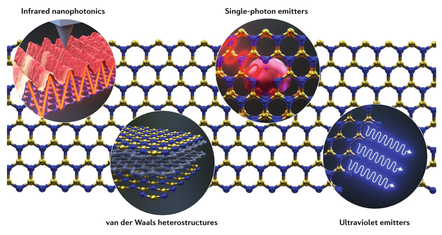
Introduction

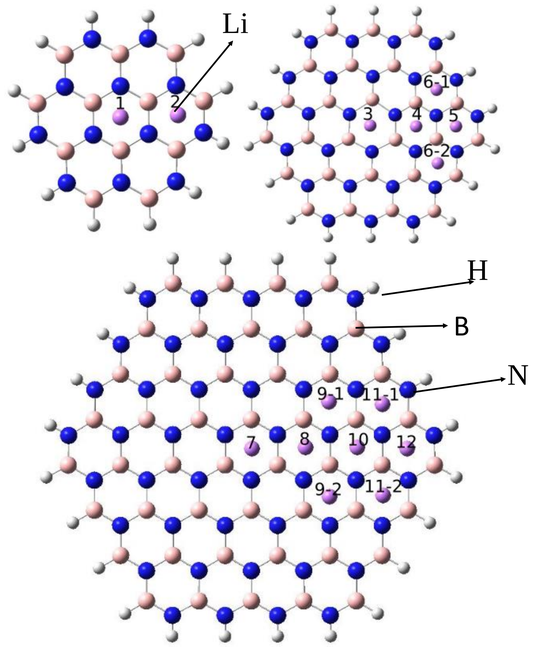




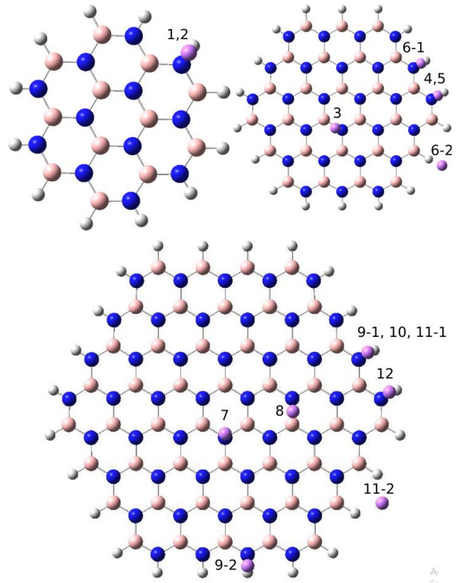


STRUCTURES & METHODS

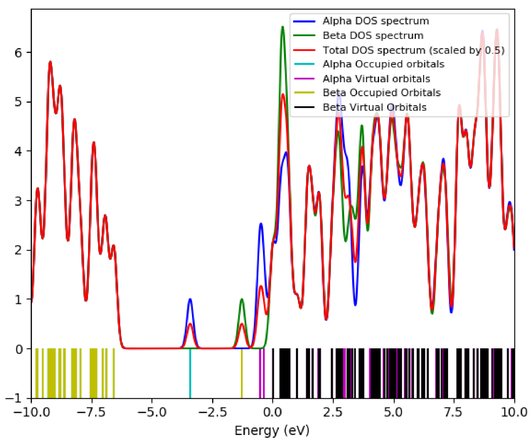
- DFT method as implemented in Gaussian 03
- B3LYP exchange-correlation hybrid function
- Polarized 6-31g(d,p) basis set



Results

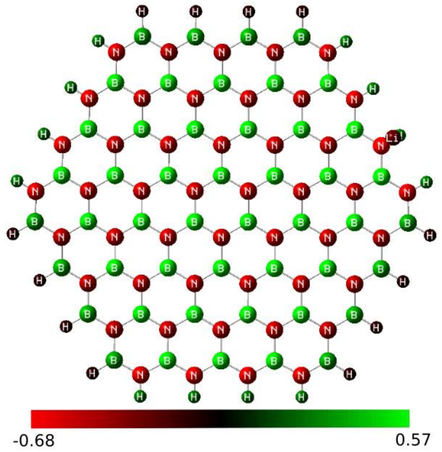


- Accordingly, for pristine flakes, stability increases as the size increases.
- For doped flakes, the adsorption energy also increases as the size increases. And, for the N-H bond adsorption, we have the maximum stability.
- The distance of the adsorbed Li atom from the BN surface decreases as the adsorption place becomes farther from the symmetry point of the BN flake. For pristine BN the bond lengths do not change as the size increases, and the changes of the bond lengths of doped BN is in order of 0.01 Å

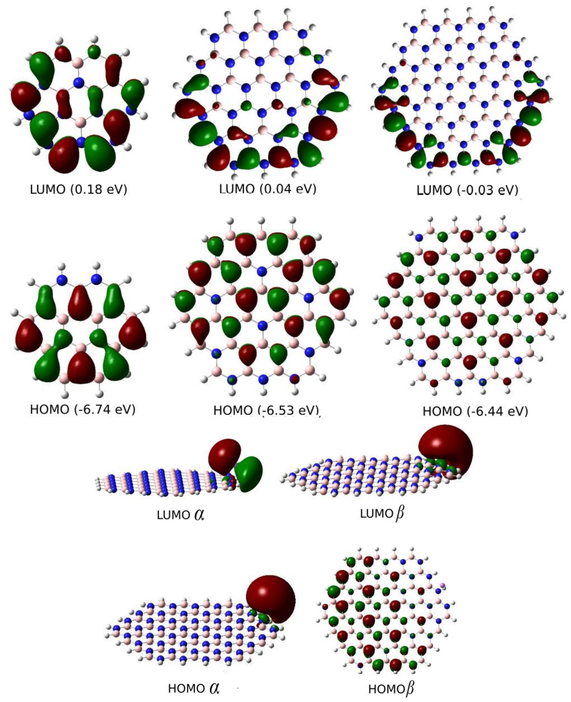


- For pristine BN, the gap increases as the size decreases. Furthermore, for doped structures, a little spin is transferred to the doped BN layer and some states are spin-polarized.
- A large value of the HOMO-LUMO gap for pristine and spin-down current leads to this point that we have a wide gap insulator for pristine BN and spin-down states. While, for spin-up electrons, the gap amounts are between 2 and 2.9 eV posses that we have a semiconductor.
- In doped cases, by the increase of the α gap, the β gap decreases.

Results

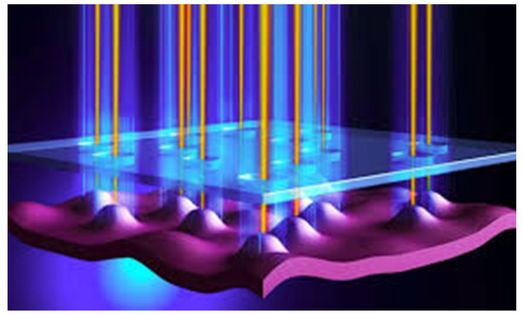


- The doped BN flakes posses non-zero dipole moments due to the asymmetry in the charge distribution.
- Edge adsorption also increases the charge interval in a cluster.
- For pristine flakes by the increase of the size, the charge distribution interval increases. In doped BN, high charge transfer from BN surface to the Li atom happens where a Li atom is adsorbed on the edge.



- For pristine BN flakes, HOMO orbitals are delocalized and those are concentrated on the N atoms. Instead, the LUMO molecular orbitals are concentrated on B atoms and MOs are localized.
- For doped structures, independent of the position of Li atom, HOMO and LUMO orbitals of spin-up states are localized, and the LUMO of spin-down electrons are localized.

Results



Conclusion

- For the first time, we have found that the adsorption of a Li atom by BN flake is possible.
- Moreover, based on the calculations, the application of BN as an insulator for a Li-ion battery is suggested.
- We have also suggested that the adsorption of a Li atom as a source of a spin defect in BN for spin-dependent photon emission devices is possible.

References

1. Kheirabadi, Narjes, and Azizollah Shafiekhani. "Intercalation of boron nitride quantum dots with Lithium: boron nitride as a protecting layer for a Lithium-ion battery and a spin-dependent photon emission device." *arXiv preprint arXiv:2006.05792* (2020).
2. Li, Lu Hua, Jiri Cervenka, Kenji Watanabe, Takashi Taniguchi, and Ying Chen. "Strong oxidation resistance of atomically thin boron nitride nanosheets." *ACS nano* 8, no. 2 (2014): 1457-1462.
3. Kheirabadi, Narjes, and Azizollah Shafiekhani. "Graphene/Li-ion battery." *Journal of Applied Physics* 112, no. 12 (2012): 124323.
4. Kheirabadi, Narjes, and A. Shafiekhani. "The ground state of graphene and graphene disordered by vacancies." *Physica E: Low-dimensional Systems and Nanostructures* 47 (2013): 309-315.

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