Hydrogen storage on cation-decorated biphenylene and nitrogenated holey carbon layered materials

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Carbon-based two-dimensional (2D) materials are becoming increasingly important for hydrogen storage due to the large surface to volume ratio and lightweight. Particularly, biphenylene (BPC) [1] and nitrogenated holey carbon (C2N) [2] are new graphene-like materials, which have been reported as a potential hydrogen storage media [3,4]. Experimental and theoretical studies have proved that metal decoration is an efficient way to increase the H_2 storage capacity. In this work, hydrogen storage on pristine and ion-decorated BPC and C_2N is addressed by dispersion-corrected density functional theory (DFT) calculations. Maximum storage capacity and adsorption energy of a gas-phase hydrogen monolayer adsorbed on both sides of pristine and ion-decorated 2D materials are investigated. Our plane-wave pseudopotential calculations were performed using the Quantum-ESPRESSO ab-initio package. Dispersive interactions were included through van der Waals exchange-correlation functional. We consider Li^+, Na^+, Mg^{2+}, Ca^{2+} ions in different concentrations adsorbed on both C_2N and BPC. Our results show that pristine BPC and C_2N can adsorbs hydrogen with modest values of binding energies and storage capacity, 0.07eV/H_2 and 4.6 wt%, respectively, similar to that found on graphene. However, ion-decorated BPC and C_2N can increase these values to ranges of -0.12 – 0.29 eV/H_2 and 6.6 – 10.3 wt%, depending on the cation species, suggesting promising applications as low-cost and lightweight H_2 storage media.

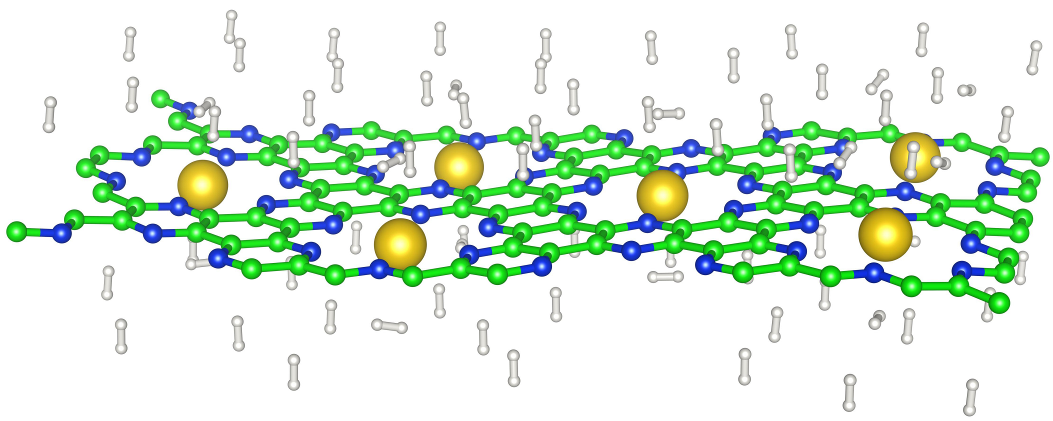

Figure 1: First layer of H_2 adsorbed on both sides of Ca^{2+}-decorated C_2N. The cations are incorporated on the centre of the C_2N holes with a binding energy of -8.86 eV/ion. The hydrogen binding energy and storage capacity are calculated to be -0.12 eV/H_2 and 8.8 wt%, respectively.

References:
[1] F. Schlütter *et al*., Angew. Chem. Int. Ed. **53**, 1538 (2014).
[2] J. Mahmood *et al*. Nat. Comm. **6**, 6486 (2015).
[3] A. Hashmi *et al*., J. Mat. Chem A **5**, 2821 (2017).
[4] R. Pan *et al*., Comput. Mat. Sci. **124**, 106 (2016).