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) \cite{1} and nitrogenated holey carbon (C2N) \cite{2} are new graphene-like materials, which have been reported as a potential hydrogen storage media \cite{3,4}. Experimental and theoretical studies have proved that metal decoration is an efficient way to increase the H\textsubscript{2} storage capacity. In this work, hydrogen storage on pristine and ion-decorated BPC and C\textsubscript{2}N 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\textsuperscript{+}, Na\textsuperscript{+}, Mg\textsuperscript{2+}, Ca\textsuperscript{2+} ions in different concentrations adsorbed on both C\textsubscript{2}N and BPC. Our results show that pristine BPC and C\textsubscript{2}N can adsorb hydrogen with modest values of binding energies and storage capacity, 0.07eV/H\textsubscript{2} and 4.6 wt\%, respectively, similar to that found on graphene. However, ion-decorated BPC and C\textsubscript{2}N can increase these values to ranges of -0.12 – 0.29 eV/H\textsubscript{2} and 6.6 – 10.3 wt\%, depending on the cation species, suggesting promising applications as low-cost and lightweight H\textsubscript{2} storage media.

Figure 1: First layer of H\textsubscript{2} adsorbed on both sides of Ca\textsuperscript{2+}-decorated C\textsubscript{2}N. The cations are incorporated on the centre of the C\textsubscript{2}N 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\textsubscript{2} and 8.8 wt\%, respectively.

References: