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Carbon Dioxide Preferential Adsorption and Conversion on Sodium Decorated γ-Graphyne

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Addressing carbon dioxide (CO_2) emissions represents a major challenge for modern society and the development of innovative and efficient technologies for CO_2 capture and conversion is paramount. Carbon materials are promising candidates for this purpose due to their versatility and sustainability and the recently synthesized[1,2] γ-graphyne 2D carbon layers are here theoretically investigated to assess their CO_2 adsorption capacity. The motivation comes from a previous validation[3] of γ-graphyne as an optimal substrate for sodium (Na) decoration with single alkali atoms hosted by each of its subnanometric pores and providing the 2D carbon layer with strongly adsorbed and positively charged metal species.

By means of a combination of finite-cluster models and periodic boundary condition DFT calculations (at the B3LYP-D3 and PBE-D3(BJ) levels, respectively) we demonstrate that Na decorated γ-graphyne layers show a significant and selective adsorption of CO_2 with respect to other representative post-combustion gas species. In particular, this occurs for a high density of Na decoration and in such cases CO_2 is adsorbed as an activated anionic species. Importantly, in this activated form CO_2 becomes very reactive and can be easily converted into sodium formate in presence of water via a highly exothermic process.

The obtained results suggest that Na-decorated γ-graphynes represent very promising adsorbing platforms based on earth-abundant elements to be used for the efficient CO_2 capture and *in-situ* conversion into added-value products.

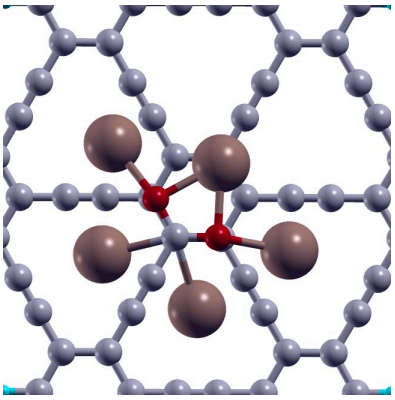

Fig. 1 CO_2 strongly adsorbed (E_{int}≅-1.9 eV) on γ-graphyne featuring a high density of sodium decoration. The molecular species is adsorbed as an anionic and activated form which can be easily converted into sodium formate.

References:

1. V.G. Desyatkin et al., *J. Am. Chem. Soc.* **144**, 17999–18008 (2022)
2. S. He et al., *Nanoscale Adv.* **5**, 2487–2492 (2023)
3. M. Bartolomei et al. *ACS Materials Letters*, **6**, 4682–4689 (2024)