

Gas Storage in Carbophenes

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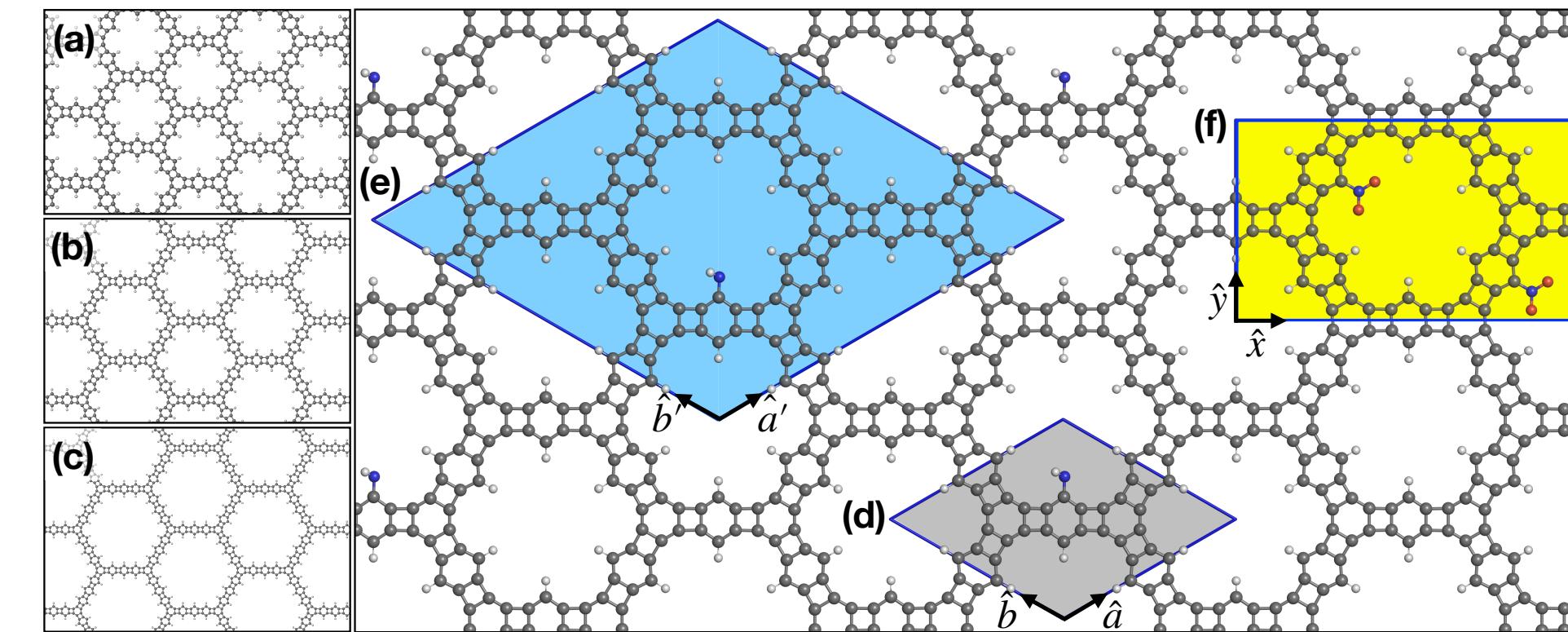
Introduction

N-carbophene's unique physical and chemical properties (e.g., conductivity and selective permeability) make this type of material an ideal candidate for several potentially valuable applications, such as carbon dioxide reduction in spacecraft, submarines, mines, and other tight spaces where it can become a breathing hazard. Leveraging computer-simulated models, our research group studied various functional groups used to calculate the absorption energy of three small molecules: H₂, CO₂, and CH₄. Employing DFTB+ calculations to analyze N-carbophene has provided clarity on its potential applications.

History of N-Carbophenes

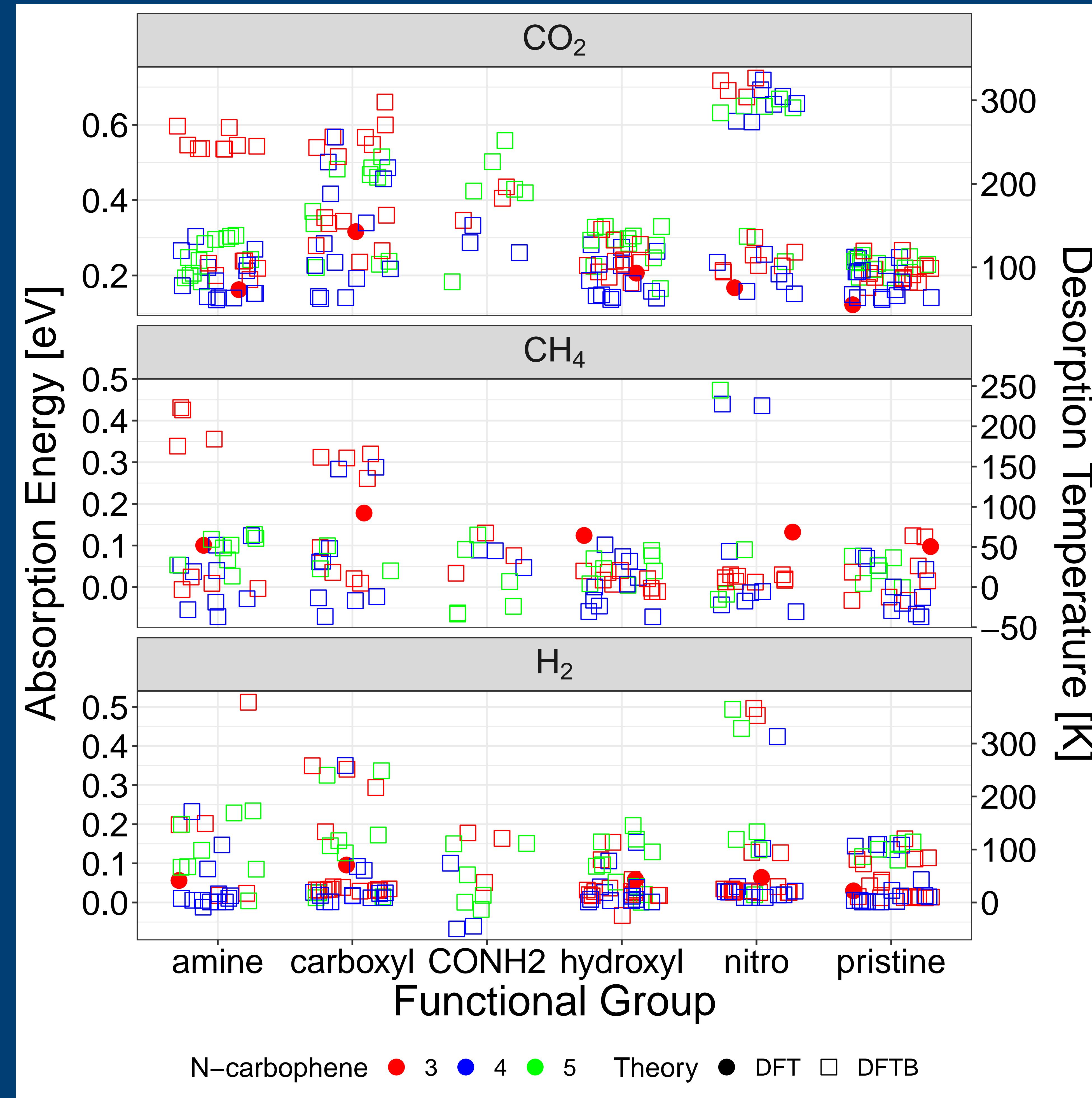
The characterization of graphene led to researchers proposing many other forms of 2D carbon, and synthesizing a few cases. In 2017, Du et al. wrote that they may have synthesized a long hypothesized type of 2D carbon: graphenylene. But Du's group had a result that suggested they may have synthesized a similar type of material called carbophene.

N-carbophene's lattice structures

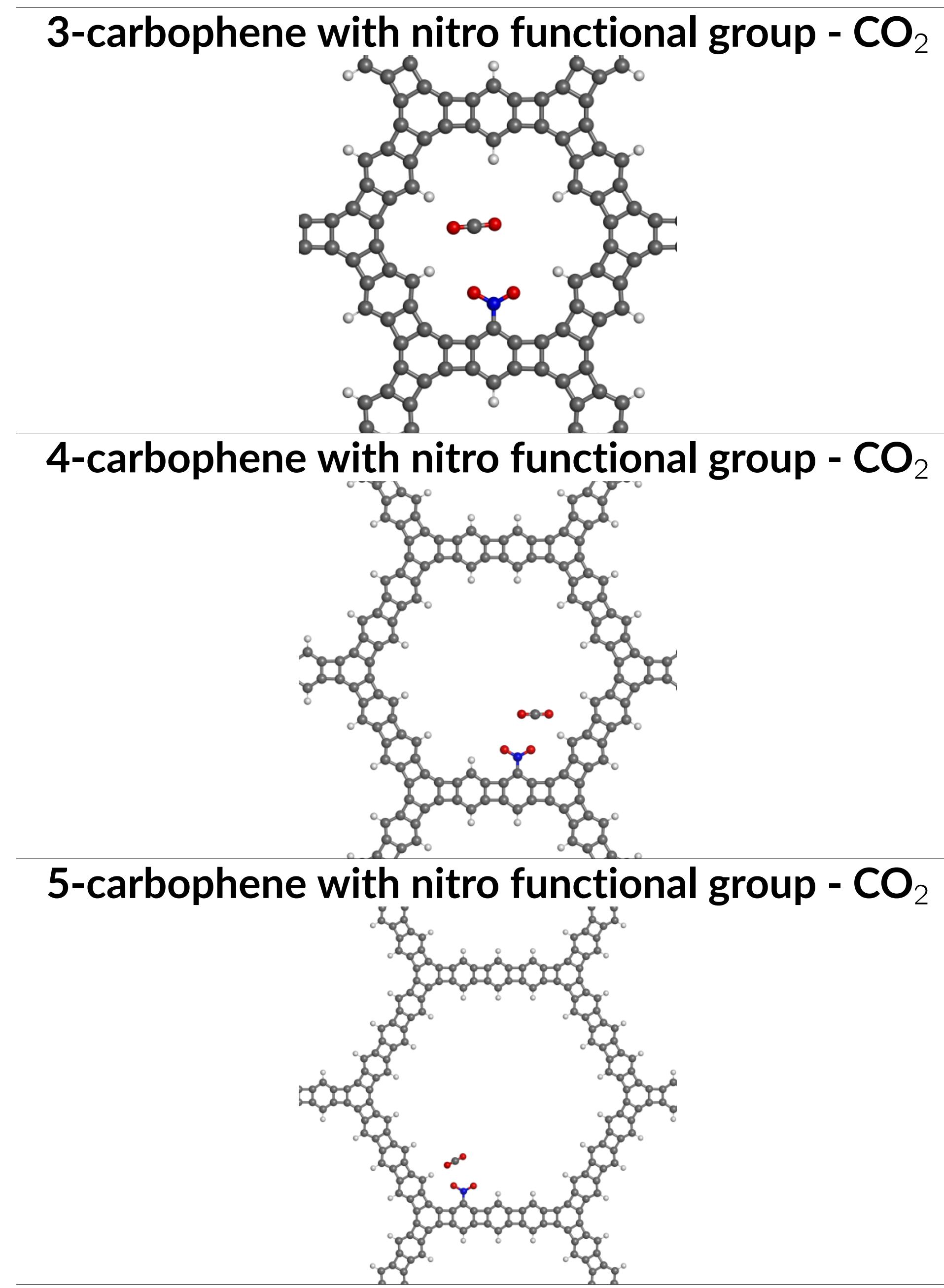


Examples of the pristine (a) 3-, (b) 4-, and (c) 5-carbophene used in this work. (d) Primitive unit cell, (e) 2-by-2 supercell (f) rectangular supercell used with ADF-BAND calculations

Absorption energies of CO₂, CH₄, and H₂



Functionalized carbophenes have larger CO₂ and CH₄ adsorption energies than other next-generation solid-state capture materials. Yet, the low predicted desorption temperatures mean that they will be beneficial as air scrubbers in confined spaces. They have H₂ adsorption energies usually observed in metal-containing materials. The predicted desorption temperatures of H₂ lie within the DOE/HST operating temperature range.



These images show results that suggest functional carbophenes contain the potential to capture small molecule gases. Specifically, the nitro group running with the adsorbate CO₂ has adsorption results of 0.695 eV, 0.659 eV, 0.649 eV for 3-carbophene, 4-carbophene, and 5-carbophene.

Conclusion

We present a study on N-carbophene, a class of 2D carbon structures composed of alternating units of cyclobutene and cyclohexatriene, explored chemically modified carbophene's potential to capture atmospheric gasses like carbon dioxide, molecular hydrogen, and methane. Nitro functional groups with the highest average adsorption energy of 0.67 eV and carboxyl functional group with average adsorption energy of 0.436 eV especially suggest higher absorption energy level. These findings offer promising avenues for developing practical solutions to capture atmospheric gases using novel carbon-derived materials.

References

