Title: Carbon Capture: theoretical guidelines of screening graphene-derived materials

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Abstract:
Discovering excellent materials for carbon capture is crucial to forge it as a viable climate change solution. Graphene is a promising material for carbon capture due to its high surface area (high capacity), its thermal and chemical stability in direct air and flue gas environments, and its well-matched physical properties. In this work, we conducted Density Functional Theory (DFT) calculations to screen various dopants, functional groups, and defects on graphene. CO2 adsorption energy, the energy required to break the bond between CO2 and the graphene derivative, is used as a metric to determine the best performing graphene-derived materials for carbon capture. Multiple studies have similarly done this work but with a narrow list of materials screened, which have ultimately yielded inconsistent results due to differing computational methods. We have constructed a clear picture of CO2 adsorption on graphene derivatives ranging from physisorption to chemisorption. Further, we established a target CO2 adsorption energy of –0.41 eV, for carbon capture and release, which is based on Mg-MOF-74 and monoethanolamine (industrial solution). Monovacancy defect graphene is near our target adsorption energy but is considered a negative as defects are difficult to control in the synthesis process. The best performers are NH2CH3 and C5H5N functionalized graphene. They are both found to be monovacancy defect insensitive and are excellent candidate materials for carbon capture.