ABSTRACT

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An effective strategy to address the climate change is to utilize Direct Air Capture (DAC) technology for seizing the legacy atmospheric CO2. The level of effectiveness depends on the selection of a suitable CO2 adsorbent that can accommodate more CO2 on its surface while consuming less energy. Organically derived biochar, a promising sustainable adsorbent, was evaluated experimentally for its innate pore structure and surface area using Brunauer–Emmett–Teller (BET) surface area analysis and its amorphous structure using powder x-ray diffraction (PXRD). Graphene served as a chemically similar substitute in quantum chemical Density Functional Theory (DFT) calculations for biochar, whose structure differs based on the source. Austin-Frisch-Petersson Functional with Dispersion (APFD) hybrid functional coupled with 3-21+g*, 6-31+G(d,p) and 6-311+G(2d,p) basis sets were employed to optimize and to calculate frequency for CO2 and finite graphene sheets in Gaussian ’16; quantum confinement and hydrogen-termination effects were investigated, and the adsorption energy was also estimated.