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Counter-Intuitive Magneto-Water-Wetting Effect to CO_2 Adsorption at Room Temperature Using $MgO/Mg(OH)_2$ Nanocomposites

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Abstract: $MgO/Mg(OH)_2$-based materials have been intensively explored for CO_2 adsorption due to their high theoretical but low practical CO_2 capture efficiency. Our previous study on the effect of H_2O wetting on CO_2 adsorption in $MgO/Mg(OH)_2$ nanostructures found that the presence of H_2O molecules significantly increases (decreases) CO_2 adsorption on the MgO ($Mg(OH)_2$) surface. Furthermore, the magneto-water-wetting technique is used to improve the CO_2 capture efficiency of various nanofluids by increasing the mass transfer efficiency of nanobeads. However, the influence of magneto-wetting to the CO_2 adsorption at nanobead surfaces remains unknown. The effect of magneto-water-wetting on CO_2 adsorption on $MgO/Mg(OH)_2$ nanocomposites was investigated experimentally in this study. Contrary to popular belief, magneto-water-wetting does not always increase CO_2 adsorption; in fact, if $Mg(OH)_2$ dominates in the nanocomposite, it can actually decrease CO_2 adsorption. As a result of our structural research, we hypothesized that the creation of a thin H_2O layer between nanograins prevents CO_2 from flowing through, hence slowing down CO_2 adsorption during the carbon-hydration aging process. Finally, the magneto-water-wetting technique can be used to control the carbon-hydration process and uncover both novel insights and discoveries of CO_2 capture from air at room temperature to guide the design and development of ferrofluid devices for biomedical and energy applications.

Keywords: room temperature; CO_2 adsorption; magneto-wetting; nesquehonite; aging

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TGA analysis was done by loading 6–7 mg to a platinum pan in the TGA unit, for CO_2 adsorption performance measurement. To avoid errors caused by pre-adsorbed species as atmospheric CO_2, water, and other impurities, samples were first pre-treated at 150 °C for 60 min under a flow of high purity N_2 (40 mL min^{-1}) with a ramp rate of 10 °C min^{-1}. The temperature was then lowered to the desired adsorption temperature at a rate of 10 °C min^{-1}, the gas was switched from N_2 to CO_2 with a constant flow of high purity CO_2 (1 atm, 40 mL min^{-1}), and the CO_2 adsorption uptake was measured for 90 min.

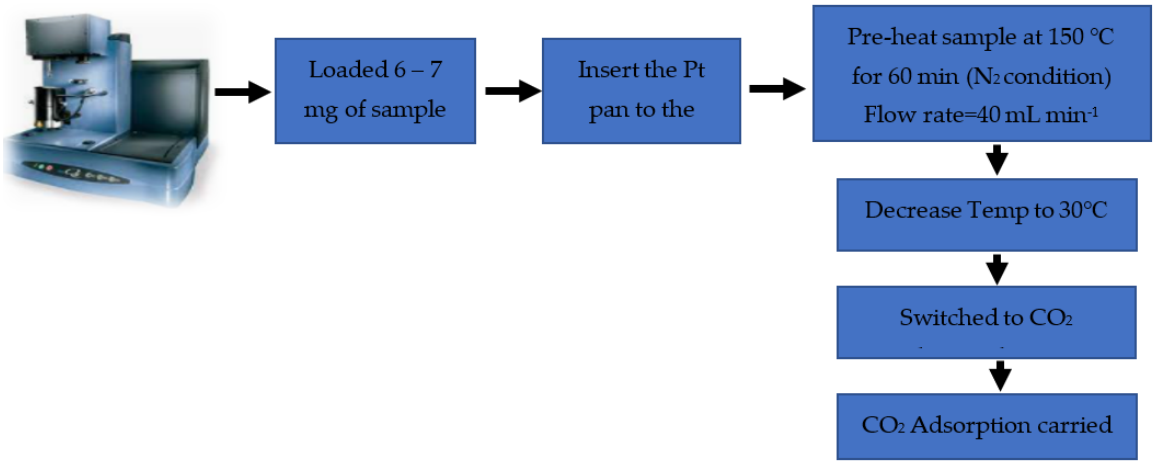

Figure S1. A schematic diagram of the TGA analysis process for the CO_2 capture capacity of the samples and figure of TGA Q50 analyser [1].

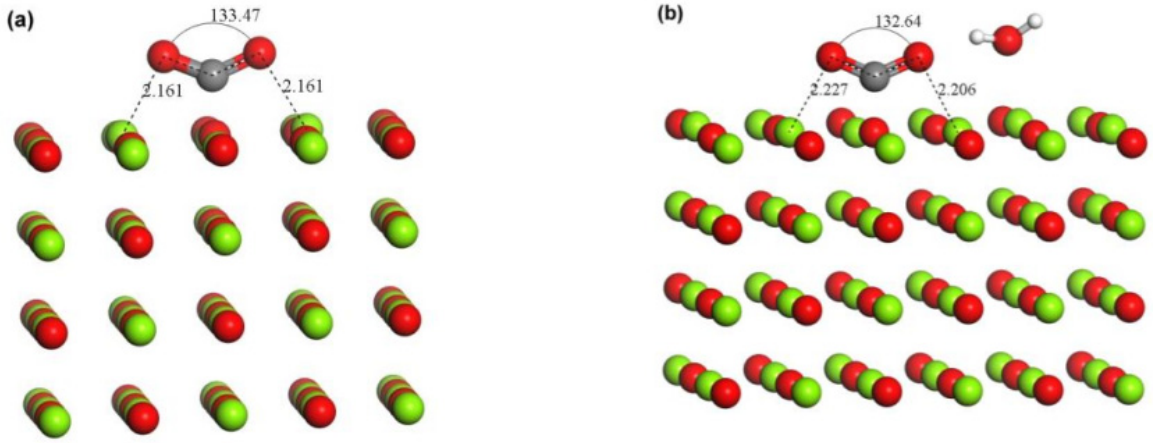

Figure S2. Optimized configuration of adsorbed CO_2 on MgO surface (**a**) and with H_2O (**b**). Atoms are shown as colored balls: hydrogen (white), oxygen (red), magnesium (green), and carbon (grey).

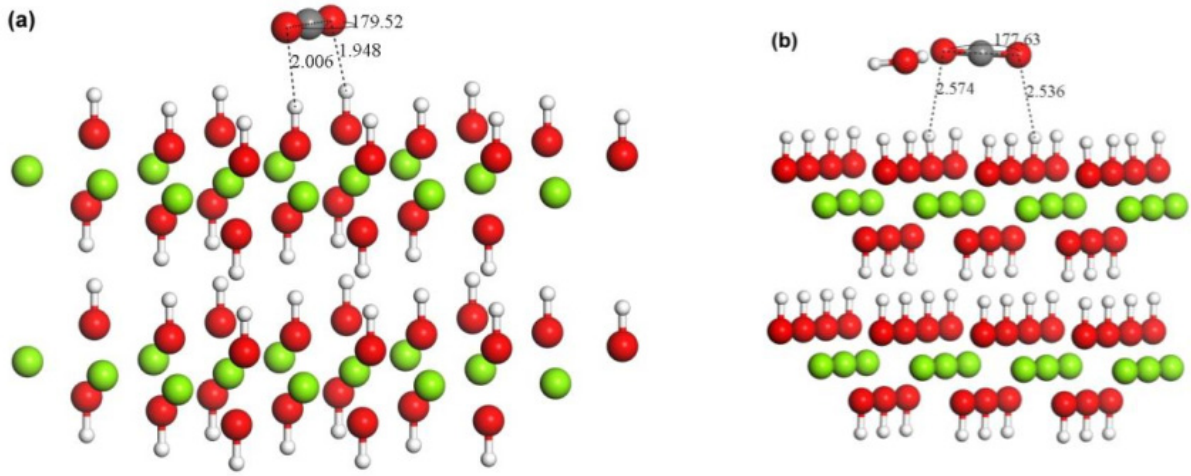

Figure S3. Optimized configuration of adsorbed CO_2 on $Mg(OH)_2$ surface (**a**) and with H_2O (**b**). Atoms are shown as colored balls: hydrogen (white), oxygen (red), magnesium (green), and carbon (grey).

Reference

1. TA Instruments. TA instruments thermogravimetric analyzers. Available online: http://www.tainstruments.com/pdf/literature/OLD_tgabrochure.pdf (accessed on 5 January 2022).