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Hydrogen Adsorption in Carbon-Based Materials Studied by NMR[1]

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Hydrogen storage is a key component for hydrogen economy. So far, storage materials with large storage capacity and suitable adsorption energy remain elusive. The identification of future storage materials depends crucially on the understanding of adsorption mechanisms. Here we show that nuclear magnetic resonance (NMR) is a sensitive and quantitative probe for detecting adsorbed gas molecules (such as H_2, methane, and ethane) in carbon-based materials [1]. Adsorbed gas molecules can be identified through characteristic NMR signatures such as spectral lineshape and spin dynamics, which is determined by the distinct dynamic properties of the adsorbed molecules. NMR is shown to be valuable for the understanding of adsorption mechanisms. In our studies, NMR measurements were carried out in-situ under given H_2 pressure up to a pressure of over 100 atm. From such ^{1}H NMR measurement, the amount of adsorbed H_2 molecules can be determined versus pressure. This gives an alternative method for measuring the adsorption isotherms where the H_2 signature is identified based on spin properties rather than weight or volume as in gravimetric and volumetric measurements. In addition, properties of molecular dynamics can be obtained at the same time providing information on the adsorption mechanisms. [1] A. Kleinhammes, S.-H. Mao, X.-J. Yang, X.-P. Tang, H. Shimoda, J. P. Lu, O. Zhou, and Y. Wu, *Phys. Rev. B.* **68**, 075418 (2003).

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