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## Analyzing the Performance of Propylamine-Grafted Mesoporous Silica for Direct Air Capture Applications

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The development of adsorbent materials for CO2 capture from the atmosphere is the focus of this study. There is a widespread agreement among scientists that greenhouse gases (GHGs) are responsible for trapping heat in the atmosphere. The concentration of CO2 in the atmosphere grew from 320 to 425 parts per million by volume (ppmv) between 1960 and 2024. According to NASA, this rise contributed to the 1.2 °C increase in average world temperature compared to the average of the late-19th century. In 2018, the Intergovernmental Panel on Climate Change (IPCC) called for a reduction of 45% in CO2 emissions by 2030, relative to the levels in 2010, to limit the global temperature increase to 1.5 °C. The Blue Map Scenario developed by the International Energy Agency (IEA) suggests various methods to reduce CO2 emissions. These strategies include shifting to renewable energy sources and putting CO2 capture technologies into action. However, most CO2 capture studies have been focused on large point sources such as power plants that run on fossil fuels. CO2 capture from the air, also recognized as direct air capture (DAC), has recently received increased attention. The United States Department of Energy acknowledges the significant contribution that DAC can make in resolving the climate challenge and moving toward the goal of reaching net-zero emissions by the year 2050. Due to their superior performance, DAC applications involving cyclic adsorption-desorption of CO2 by amine-functionalized silica materials (also known as "aminosilica") have received great attention from both the scientific community and industry. Most relevant research concentrates on near-equilibrium CO2 adsorption while adsorbent stability and adsorption kinetics are considered secondary factors in many studies. While the stability of aminosilicas determines their operational lifetime, it is vital to have fast adsorption kinetics to increase the amount of CO2 captured over a given time. This study aims to employ a novel approach by emphasizing adsorbent stability and rapid adsorption kinetics more than adsorption uptake to create aminosilicas that are highly effective and long-lasting in DAC applications. Aminosilicas were synthesized by utilizing mesoporous silica that is commercially available (CARiACT G-10, Fuji Silycia). The amine functionalization of silica was completed via grafting instead of impregnation to enhance adsorption kinetics and long-term stability of the adsorbent. Amine grafting was conducted using isolated primary amines (i.e., 3-aminopropyltrimethoxysilane; APTMS). Thermogravimetric analysis (TGA) was performed on all the materials to quantify amine loading, equilibrium CO2 uptake, amine efficiency, and CO2 adsorption kinetics in the presence of dry CO2 (400 ppmv, balance nitrogen) at an adsorption temperature of 25 °C. Selected performant materials were further investigated regarding cyclic adsorption-desorption performance, long-term thermal and oxidation stability, and columnbreakthrough experiments in the presence of dry and humid gas streams. Our preliminary results indicated that propylamine-grafted silica materials achieved a delicate balance between enhancing CO2 uptake, improving adsorption kinetics, and securing thermal and oxidation stability.

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