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Selective Adsorption of Carbon Dioxide from Mixed Vapors by Blockage of Methane in Graphene Nanoribbons

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Abstract

We propose a substrate designed to filter CO2 from a vapor mixture of CO2 and CH4 at room temperature. The technique combines energetic, kinetic and steric aspects of adsorption. The substrate consists of an array of graphene nanoribbons (GNRs) placed over graphite. Our study is based on Molecular Dynamics (MD) simulations. Methane is considered a spherical molecule and carbon dioxide is represented as a linear rigid body. Graphite is modeled as a continuous material, while the GNRs are approached atomistically. We explore the effect on the selectivity of the type of GNRs' edges, the distance between GNRs and the graphite surface, and the gaps between GNRs.

For narrow gaps (~ 7˚A openings), we show that the molecules of methane are blocked out, while CO2 molecules are able to diffuse and be collected in between the nanoribbons and the graphite surface. In this way the selectivity of CO2 is extremely high. For wider gaps (~ 14˚A openings) we obtain high selectivity when the GNRs are placed 6˚A above the graphite surface. In this last case, the initial rate of adsorption of CO2 is much faster than CH4. For zigzag-edged GNRs, CO2 adsorbs 19 times faster than CH4, and for armchair-edged GNRs the relative rate of adsorption is 14. Overall we show that the filter can be optimized by controlling the gap opening between the GNRs from a mixture using different substrates such as Graphene Nanoribbons and Graphite.

Biography:

Hind Aljaddani has completed her Ph.D. from Howard University in Washington DC on 28 July 2019. She is now an assistant professor at the University of Jeddah in the Kingdom of Saudi Arabia. Hind interested in the selective toxic molecule

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