

Public Abstract

First Name:Monika

Middle Name:Renata

Last Name:Golebiowska

Adviser's First Name:Carlos

Adviser's Last Name:Wexler

Co-Adviser's First Name:

Co-Adviser's Last Name:

Graduation Term:SP 2011

Department:Physics

Degree:MS

Title:THE REVERSIBILITY OF THE ADSORPTION OF METHANE-METHYL MERCAPTAN MIXTURES IN NANOPOROUS CARBON

Methane is the main constituent of natural gas (NG). As fuel for vehicular applications NG requires sorbents that allow efficient, reversible and safe storage at room temperature and moderate pressure. To enable easy human detection of gas leaks the fuel gas should be added with compounds having low odor threshold, such as thiols (mercaptans). Thus a full understanding of the behavior of methane-mercaptan mixtures is necessary for the development of safe storage systems.

In this work we present results of molecular dynamics simulations in the temperature range 198 K and 320 K and for a large range of methane partial pressures, up to the saturation pressure of methane. We observe the presence of 2D (and to a lesser degree 3D) diffusion of the thiols indicating that though thiols adsorb preferentially relative to methane, the adsorption is still reversible. We estimate that only a small increase in mercaptan concentration is necessary for the desorbed phase to be above the threshold for human detection.