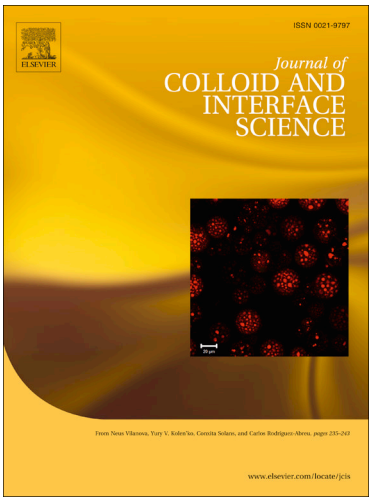

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PII: S0021-9797(18)30268-6
DOI: https://doi.org/10.1016/j.jcis.2018.03.026
Reference: YJCIS 23376

To appear in: *Journal of Colloid and Interface Science*

Received Date: 7 December 2017
Revised Date: 19 February 2018
Accepted Date: 10 March 2018

Please cite this article as: V. Cornette, J.C. Alexandre de Oliveira, V. Yelpo, D. Azevedo, R.H. López, Binary Gas Mixture Adsorption-Induced Deformation of Microporous Carbons by Monte Carlo Simulation, *Journal of Colloid and Interface Science* (2018), doi: https://doi.org/10.1016/j.jcis.2018.03.026

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ABSTRACT

Considering the thermodynamic grand potential for more than one adsorbate in an isothermal system, we generalize the model of adsorption-induced deformation of microporous carbons developed by Kowalczyk et al. [1]

We report a comprehensive study of the effects of adsorption-induced deformation of carbonaceous amorphous porous materials due to adsorption of carbon dioxide, methane and their mixtures. The adsorption process is simulated by using the Grand Canonical Monte Carlo (GCMC) method and the calculations are then used to analyze experimental isotherms for the pure gases and mixtures with different molar fraction in the gas phase. The pore size distribution determined from an experimental isotherm is used for predicting the adsorption-induced deformation of both pure gases and their mixtures. The volumetric strain (ε) predictions from the GCMC method are compared against relevant experiments with good agreement found in the cases of pure gases.

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1. INTRODUCTION

Gas adsorption in porous solids is known to induce elastic deformation, and this is well-documented in the literature, dating back to the first experimental evidence of swelling of charcoal by Meehan[2] and Bangham and co-workers[3] in the late 1920s. In