

Simulations of Phenol Adsorption onto Activated Carbon and Carbon Black[†]

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ABSTRACT: Grand canonical Monte Carlo (GCMC) and molecular dynamics (MD) simulations have been used to study the adsorption of phenol onto carbon materials. Activated carbon was modelled in terms of its pore-size distribution based on DFT methods, while carbon black was represented by a single carbon slab with varying percentages of surface atoms removed. GCMC results for adsorption from the corresponding gas phase were in reasonable agreement with experimental adsorption results. MD simulations, that studied the influence of the presence of water and surface roughness on the arrangement of the adsorbed phenol molecules, showed that the interaction between the adsorbed molecules was strongly influenced by the presence of water.

1. INTRODUCTION

The adsorption of phenol onto activated carbon has attracted much experimental interest due to the importance of removing this pollutant from water and air. However, the adsorption of phenol onto carbon materials is a complex process and the number of studies which have investigated the interaction of phenol with carbon surfaces by simulation is still limited. Bertonecini *et al.* (2000, 2003) performed grand canonical Monte Carlo (GCMC) simulations of phenol onto porous and non-porous carbons from the gaseous phase. By comparing the simulated results with experimental liquid adsorption data, these authors concluded that the solvent effect was negligible.

Efremenko and Sheintuch (2006) used DFT and molecular mechanics simulations of phenol on flat carbon surfaces and in carbon nanopores. Due to the small clusters investigated by DFT, the adsorption of molecules was restricted to a small number (up to five molecules adsorbed directly onto the surface, whereas the sixth molecule was adsorbed in the second layer). The effect of functional groups on the interaction was also included in this study. Molecular mechanics simulations were also employed by Abir and Sheintuch (2010). The results obtained for single-wall carbon nanotubes were used to predict the adsorption isotherms for carbons with pore-size distributions.

Terzyk *et al.* (2010) examined phenol adsorption from solution onto virtual porous carbons with different pore-size distributions by molecular dynamics (MD) simulations and studied the effect of oxygen modifications. However, no comparison with experimental data was undertaken in this study.

The work presented here describes further investigations of the adsorption of phenol onto carbon materials with a focus on the effect of water. This has been undertaken in two ways: (1) by