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Molecular Dynamics Simulation of Realistic Biochar Models with Controlled Microporosity

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Abstract : Biochar is an amorphous carbon-rich material generated from the pyrolysis of biomass with multifarious properties and functionality. Biochar has shown proven applications in the treatment of flue gas and organic and inorganic pollutants in soil and water/wastewater as a result of its multiple surface functional groups and porous structures. These properties have also shown potential in energy storage and carbon capture. The availability of diverse sources of biomass to produce biochar has increased interest in it as a sustainable and environmentally friendly material. The properties and porous structures of biochar vary depending on the type of biomass and high heat treatment temperature (HHT). Biochars produced at HHT between 400°C – 800°C generally have lower H/C and O/C ratios, higher porosities, larger pore sizes and higher surface areas with temperature. While all is known experimentally, there is little knowledge on the porous role structure and functional groups play on processes occurring at the atomistic scale, which are extremely important for the optimization of biochar for application, especially in the adsorption of gases. Atomistic simulations methods have shown the potential to generate such amorphous materials; however, most of the models available are composed of only carbon atoms or graphitic sheets, which are very dense or with simple slit pores, all of which ignore the important role of heteroatoms such as O, N, S and pore morphologies. Hence, developing realistic models that integrate these parameters are important to understand their role in governing adsorption mechanisms that will aid in guiding the design and optimization of biochar materials for target applications. In this work, molecular dynamics simulations in the isobaric ensemble are used to generate realistic biochar models taking into account experimentally determined H/C, O/C, N/C, aromaticity, micropore size range, micropore volumes and true densities of biochars. A pore generation approach was developed using virtual atoms, which is a Lennard-Jones sphere of varying van der Waals radius and softness. Its interaction via a soft-core potential with the biochar matrix allows the creation of pores with rough surfaces while varying the van der Waals radius parameters gives control to the pore-size distribution. We focused on microporosity, creating average pore sizes of 0.5 - 2 nm in diameter and pore volumes in the range of 0.05 – 1 cm3/g, which corresponds to experimental gas adsorption micropore sizes of amorphous porous biochars. Realistic biochar models with surface functionalities, micropore size distribution and pore morphologies were developed, and they could aid in the study of adsorption processes in confined micropores.

Keywords : biochar, heteroatoms, micropore size, molecular dynamics simulations, surface functional groups, virtual atoms
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