Molecular simulations of confined deep eutectic solvents for gas separations and liposomes for drug delivery

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Abstract

This dissertation leverages molecular dynamics simulations to explore the properties of nanoscale materials and interfaces involving gases, liquids and solids, traversing the realms of environmental and biological science. This work not only demonstrates the expansive applicability of MD simulations across various scientific disciplines but also highlights their capability to provide profound insights into diverse scientific phenomena.

In the segment dedicated to deep eutectic solvents, our study investigates the behavior of ethaline (mixtures of choline chloride with ethylene glycol at different molar ratios) confined in graphite and titania (rutile) slit pores, measuring 2 nm and 5 nm in width. This research aims to address the high viscosity issue prevalent in these solvents when saturated with CO2. The results reveal that modifications in the ethylene glycol ratio, variations in pore sizes, and the choice of pore wall materials significantly affect the efficiency of CO2/CH4 separation. These findings offer a deeper understanding of how molecular interactions and structural changes in confined spaces can influence the physical properties of DES.

The dissertation also delves into the domain of liposomes (nanoparticles formed by a lipid bilayer encapsulating an aqueous core), examining the influence of lipid composition

and the integration of two distinct small-molecule hydrophobic drugs on their mechanical, spatial, and fluid properties. The study encompasses an analysis of the effects of acyl chain saturation and length, diverse lipid headgroups, and drug incorporation. Experimental validations, conducted in collaboration with Prof. Auguste's laboratory, support our simulation findings. We discovered that lipids with short-saturated acyl chains and varied headgroups alter the lipid bilayer packing, resulting in decreased liposome stiffness, which has been shown promoted drug delivery efficiency. Additionally, specific drug substances were observed to lower interaction energies within the lipid matrix, which consequently reduces stiffness and enhances lipid molecule diffusion. This segment of the dissertation provides crucial insights into the design of liposomal formulations, particularly for drug delivery purposes, by demonstrating how lipid structure and drug interactions can be manipulated to optimize liposome properties.

Overall, this dissertation underscores the versatility of molecular dynamics simulations in elucidating complex material behaviors and offers valuable contributions to the various engineering fields.