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Molecular dynamics simulation on self-diffusion coefficients of CO_2 in substituted amines

Qu Chen*, Yanping Tang, Xiaojuan Ji

Zhejiang University of Science and Technology, Hangzhou, People's Republic of China

*Presenting author: quchen@zju.edu.cn

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Carbon Capture and Storage has been one of the essential routes to reduce carbon emission from power plants. In the well-known post-combustion process to generate electricity, a large amount of CO_2 is produced in a relatively low pressure so that an amine-based chemical solvent is ideal for the acid gas removal. So far, a number of amines have been identified for commercial use including monoethanolamine (MEA), diethanolamine (DEA), N-methyldiethanolamine (MDEA), dimethylmonoethanolamine (DMMEA), diisopropanolamine (DIPA), diethylenetriamine (DETA), tetraethylenepentamine (TEPA), 2-amino-2-methyl-1-propanol (AMP), and piperazine (PZ). However, for the rational design of reaction facilities, it is very important to understand the transport properties of CO_2 in the above-mentioned solvents. In industry, however, CO_2 can readily react with amines, so the CO_2/N_2O analogy has been extensively used to calculate the diffusivity of CO_2 in chemical solvents. Alternatively, computer simulation is a powerful tool, which can automatically "switch off" the reaction between CO_2 and amines so that the transport properties of CO_2 can be directly computed. In this work, we seek to build reliable force-fields for all the amines, calculate the diffusivity of CO_2 in these chemical solvents, discuss the implications of the computed diffusivities, and validate the CO_2/N_2O analogy in amine-based solutions. This work may provide insights into the choice of amine solutions for industrial use.

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