Keynote Lecture KL 01

Clean, High Quality Low Emission Fuels with Fischer-Tropsch Synthesis: A Multiscale Study of Transport Properties in Confined Systems

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Abstract (less than 300 words)

The Fischer-Tropsch (FT) route is a polymerization reaction used extensively in the Gas-to-Liquids (GTL) process to transform synthesis gas into high quality low emission transportation fuels. The main FT reaction products, namely water, wax and small amounts of oxygenates (e.g. alcohols < 10 wt %), form a mixture through which the dissolved reactants diffuse, reach the catalytic nanoparticles and react. Key factors in ensuring FT reactor's activity and stability is the selection of the catalyst (e.g. Co) and the support material (e.g. TiO_2, Al_2O_3, graphene). Unfortunately, FTS catalysts deactivate over time and the role of oxygenates and excess water in the loss of catalyst activity remain as open questions.[1]

In order to gain a better understanding of the phase behavior of confined wax – water – alcohol mixtures in either hydrophilic or hydrophobic environment at reaction conditions, our efforts concentrated on the the *n*-C_{28} – H_2O – 1-dodecanol mixture at 473.15 K inside pristine graphene (G) and graphene oxide (GO) pores by means of Coarse Grained Molecular Dynamics (CGMD) simulations. Our simulations show that CG approaches capture the mixture phase separation and individual component diffusivity. The Co NP does not affect the mixture phase separation but it is extensively covered by water. Our results showcase that CGMD can be employed to study FTS related processes at this scale [2,3] and are expected to open new pathways in the investigation of the effect of NPs on catalyst support interfaces in the presence of FTS relevant mixtures.

References

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