

Force field based GCMC simulation for characterisation of adsorption and separation in MOFs

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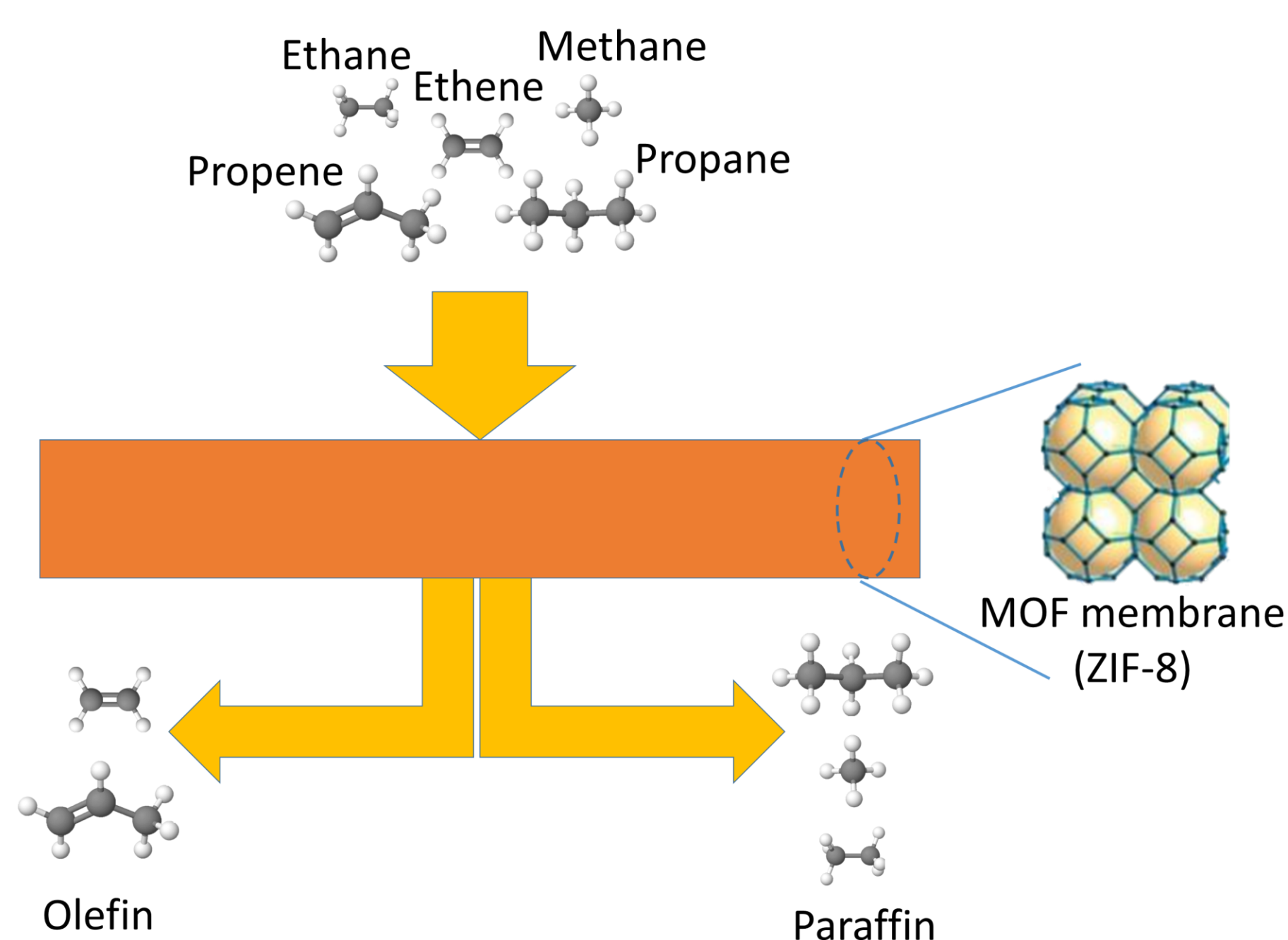
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Abstract

ZIFs are attractive candidates for membrane materials for separation of olefins and paraffins. Experimental characterization of adsorption/separation properties of MOFs is infeasible for screening large numbers of MOFs for new applications. Force-field based GCMC simulations offer a quicker alternative. However, the reliability of the predictions depends heavily on the accuracy of the force field used.

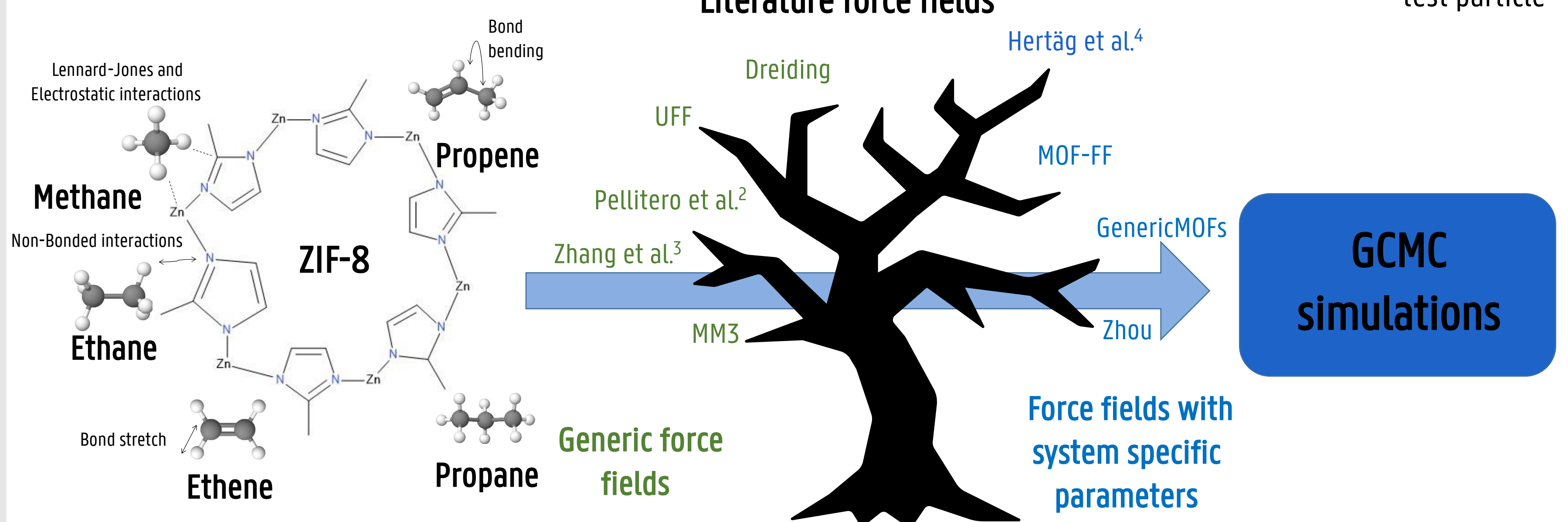
Motivation

- Olefin/paraffin separation through cryogenic distillation is energy intensive and expensive
- Membrane separation is a viable alternative
- MOFs from ZIF family are favoured due to their superior separation performance for hydrocarbon mixtures¹



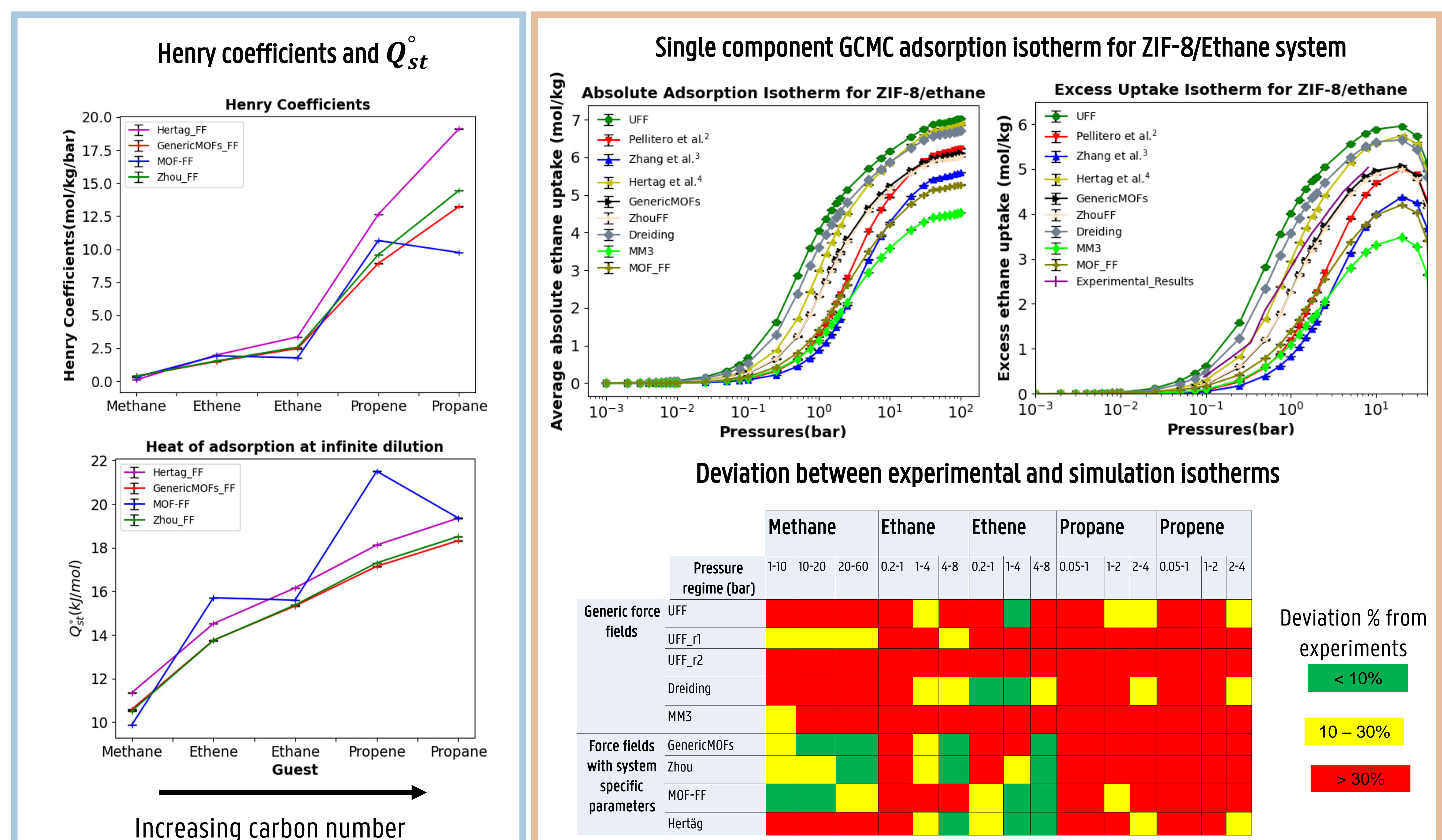
Methods

- Grand Canonical Monte Carlo Simulations (GCMC) using RASPA software package
- Widom insertion method is used for computation of Henry coefficients and heat of adsorption at infinite dilution (Q_{st}^0)



Results

- Hydrocarbons with greater carbon number contain a larger number of non-aliphatic sites and thus possess a stronger affinity with ZIF-8
- Simulation isotherms have lower deviations with experimental isotherms for hydrocarbons with lower carbon number
- Force fields with system specific parameters perform better having lower deviations with experimental isotherms on average as compared to generic force fields



- ## Outlook
- Consideration of ab initio based force fields to achieve better accuracy for hydrocarbons with larger carbon number
 - Employing ideal adsorbed solution theory (IAST) model to characterize separation properties from single-component adsorption isotherms and validation with multi-component adsorption isotherms