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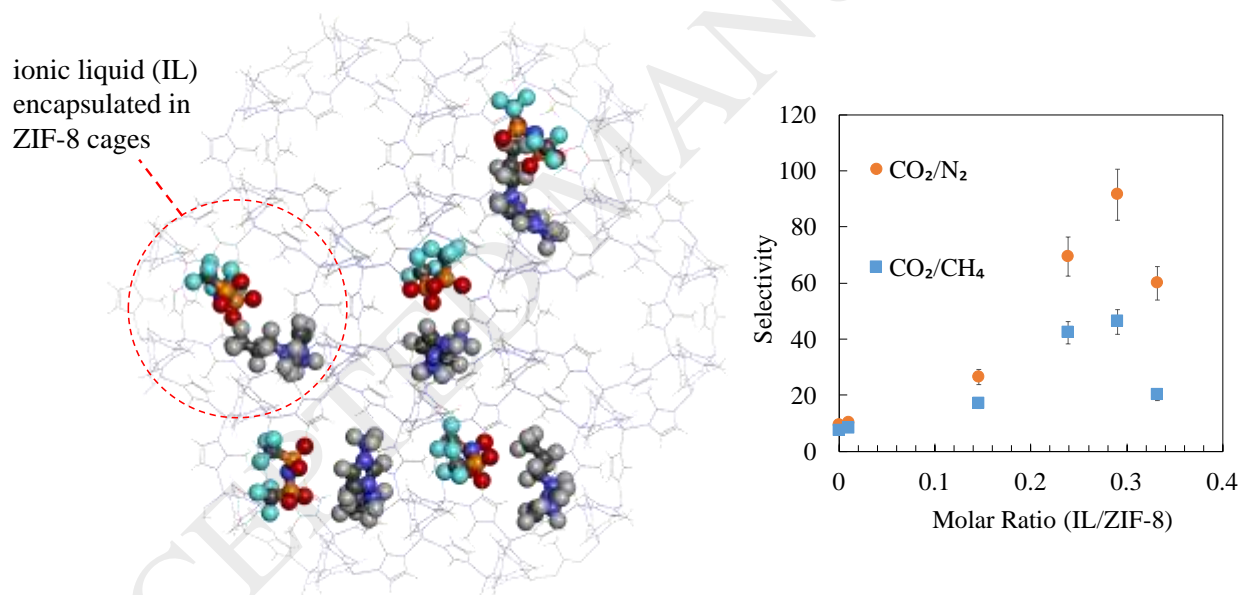
# CO<sub>2</sub> selective metal organic framework ZIF-8 modified through ionic liquid encapsulation: a computational study

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## Graphical abstract



## Highlights

- Investigation of the encapsulation of [bmim<sup>+</sup>][Tf<sub>2</sub>N<sup>-</sup>] ionic liquid (IL) in ZIF-8 as means of tailoring ZIF gas separation efficiency.
- Monte Carlo simulations to study the adsorption-based separation in ZIF-8 and the complex of ZIF-8 with the encapsulated IL pairs.
- Dramatic increase in CO<sub>2</sub> capacities and selectivities due to the IL presence.
- Determination of the optimum IL composition on CO<sub>2</sub> selectivity.

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