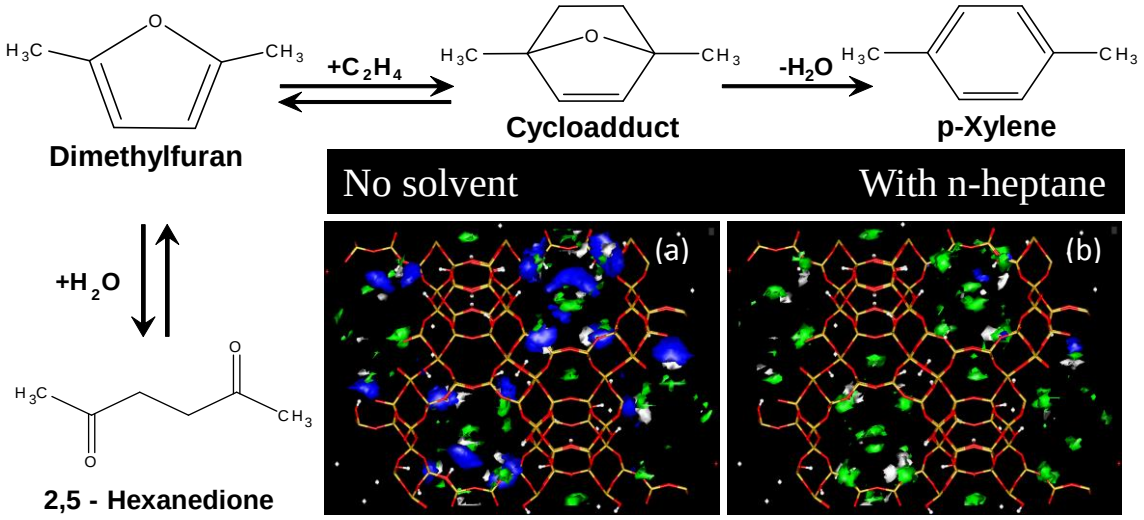
Driving up the Yield of Para-Xylene

Scientific Achievement

We performed molecular simulation to understand the role of solvent in the production of renewable p-xylene, a key monomer for green plastics.

Significance and Impact

- Solvents play a critical role in biomass processing but their mechanism is poorly understood. Molecular modeling revealed that the solvent can vary the effective hydrophobicity of microporous materials. This approach provides a strategy to rationally predict solvents and improve yield.



H-Y zeolite (Si/Al=2.6); DMF (white); Ethylene (green); Water (blue); PX (not shown)

Xiong, R.C.; Sandler, S.I.; Vlachos, D.G.; Dauenhauer, P. J., *Green Chem.* 2014, 16, 4086-4091.

Research Details

- Configurational biased Monte Carlo simulations were preformed for multicomponent systems of p-xylene production.
- Hydrophobic solvents expel water and thereby reduce hydrolysis of DMF and improve selectivity.

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Work was performed at the Univ. of Delaware and Massachusetts led by Sandler's, Vlachos' and Dauenhauer's groups