

## Microscopic origins for the favorable solvation of carbonate ether copolymers in carbon dioxide

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### Abstract

The strong desire for the wide use of carbon dioxide as an environmentally benign process solvent has spurred a large number of attempts to improve its solubility characteristics. Pioneering experimental work by Beckman and co-workers has pointed to carbonate ether copolymers as promising candidates for non-fluorous surfactants. It is demonstrated here that Gibbs ensemble Monte Carlo simulations (using configurational-bias and double-bridging strategies and the transferable potentials for phase equilibria force field) can be employed to accurately predict the phase equilibria of a carbonate ether copolymer with CO<sub>2</sub>. The simulations indicate that the greater accessibility of the carbonyl oxygen plays a major role for the CO<sub>2</sub>-philicity of this copolymer surfactant.

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