Efficient ionic liquid-based platform for multi-enzymatic conversion of carbon dioxide to methanol - DTU Orbit (07/03/2019)

Low yields commonly obtained during enzymatic conversion of CO₂ to methanol are attributed to low CO₂ solubility in water. In this study, four selected ionic liquids with high CO₂ solubility were separately added to the multi-enzyme reaction mixture and the yields were compared to the pure aqueous system (control). In an aqueous 20% [CH][Glu] system, yield increased ca. 3.5-fold compared to the control (ca. 5-fold if NADH regeneration was incorporated). Molecular dynamics simulation revealed that CO₂ remains for longer in a productive conformation in the enzyme in the presence of [CH][Glu], which explains the marked increase of yield that was also confirmed by isothermal titration calorimetry – lower energy (ΔG) binding of CO₂ to FDH. The results suggest that the accessibility of CO₂ to the enzyme active site depends on the absence/presence and nature of the ionic liquid, and that the enzyme conformation determines CO₂ retention and hence final conversion.
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