Contribution ID : **218** Type : **Poster Presentation**

Water assisted Interfacial Polymerization of TEPA and HMDI at the Water/Hexadecane Interface

Interfacial polymerization (IP) between tetraethylenepentamine (TEPA) and 4,4'-methylenebis(cyclohexyl isocyanate) (HMDI) at the water/hexadecane interface proceeds too rapidly to effectively control reaction kinetics or tailor polymer morphology. To elucidate the underlying mechanism, we performed quantum mechanical (QM) calculations, molecular dynamics (MD) simulations, and experimental verification. QM results reveal that a single water molecule significantly lowers the proton transfer energy barriers to 3.6, 4.0, 4.4 kcal/mol, compared to 15.5, 17.8, 23.9 kcal/mol of direct proton transfer (in vacuum, implicit hexadecane, and implicit water). Acting as a proton transfer bridge, the water molecule forms hydrogen bonds with both TEPA and HMDI, thereby facilitating the reaction at the interface. MD simulations show preferential adsorption of HMDI at the interface and high solubility of TEPA in water. Experimental data further confirm that polymerization occurs mainly in the hexadecane phase near the interface. This study provides the first direct evidence for water-mediated catalysis in interfacial polymerization and offers a foundation for designing better-controlled IP systems with tunable morphology and kinetics.

Primary author(s) : Dr. LIU, Biyuan (California Institute of Technology); Dr. ZHANG, Yonglin; ZHAO, Ying; PRABHAT, Prakash; HUAI, Liyuan; MA, Hancheng; LUO, Zhengtang; A. GODDARD III, William; YANG, Jinglei

Presenter(s) : Dr. LIU, Biyuan (California Institute of Technology)