Porous Organic Polymer via Catalyst free Diels-Alder Cycloaddition

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The aim of this work was the synthesis and characterization of two newly developed fully sp^2-Hybridized Porous Organic Polymers (POPs) with potential applications in water capture, gas absorption, lithium ion uptake and electron conductivity. The three- and two-dimensional polymers are the Catalyst Free Diels-Alder Cycloaddition polymerization product of Bisbenzyne and Cyclooctatetrafuran, Cyclohexatrifuran respectively. The energy difference of the Molecular Orbitals (MOs) involved in the Diels-Alder cycloaddition reaction were calculated using Density Functional Theory (DFT) B3LYP/6-311++G** and resulted in a relative estimation of the reaction kinetics. The polymerization reaction was verified by Fourier-Transformed Infrared (FT-IR) spectroscopy confirming the incorporation of the Furan and Benzene unit inside the polymer structure. The lattice distance was determined by Powder X-Ray Diffraction (PXRD) analysis resulting in 4.8 Å for the 3DPOP and 4.7 Å for the 2DPOP. The high oxygen content inside the polymer structure allow hydrogen bonding with water molecules, hence rendering them attractive as dehumidifier. The atmospheric water capture capacity was investigated and resulted in 19% (w/w) and 21% (w/w) for the 3DPOP, 2DPOP respectively. These results indicate an efficiency comparable to commercial desiccants such as zeolites 22-30% (w/w) and activated alumina 19% (w/w). Furthermore, Scanning Electron Microscopy (SEM) images were recorded in order to investigate the morphology of the polymers.

Overall, the fully sp^2-hybridized Porous Organic Polymers synthetized in this work are very promising for water capture and gas absorption.
Furthermore, the polymers are interesting precursors for conjugated aromatic polymers with potentially high lithium ion uptake and electron conductivity.

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