Abstract Submitted
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Ab-initio study of polypyrrole as a pervaporation membrane ANDRE BOTELHO, XI LIN, Boston University — The affinities between polypyrrole, water, ethanol and a sulfonate-carrying ion were calculated from first principles. All interactions were demonstrably hydrogen bonds between the oxygen from the sulfonate groups and the hydrogen in the hydroxyl (for water and ethanol) and amine groups (for polypyrrole). Each sulfonate group was shown to form three hydrogen bonds, with any of the three other types of molecules, allowing the ion complex to bind to multiple polypyrrole chains, water, and ethanol molecules simultaneously. The energies indicated a higher affinity between the ion and poypyrrole, second highest between water and the ion, and the lowest for ethanol and the ion. A high affinity of the ion to the polymer backbone is desirable to prevent leeching. The ion was found to have a higher affinity to water molecules than to ethanol, confirming the system's selectivity in separating water from ethanol.

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