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Type: **Poster Presentation**

## **Computational study of the effect of polydimethylsiloxane (PDMS) side chain size and spacing on the mobility of the polyethylene oxide (PEO).**

*Wednesday, 13 July 2011 17:00 (2 hours)*

The effects of side chain size and spacing on the mobility of the PEO backbone have been studied using molecular dynamics (MD) in Forcite code of Materials studio. The systems investigated contain a PEO chain of 186 ethylene oxide (EO) monomers to which side chains of 5, 6, 7, 8 and 9 PDMS monomers have been attached. The separations of the side chains used are 5, 10, 15, 20 and 50 EO monomers. The overall mobility of the polymer host system is found to have minima at side chain size of 6 and 7. A maximum is seen at side chain spacing of 8 and 9. No evident was found to suggest that side chain spacing has an effect on the mobility of the PEO polymer backbone. Furthermore, the point of attachment of the side chain has no effect on the polymer mobility.

**Level (Hons, MSc, <br> &nbsp; PhD, other)?**

PhD

**Consider for a student <br> &nbsp; award (Yes / No)?**

No

**Would you like to <br> submit a short paper <br> for the Conference <br> Pro-ceedings (Yes / No)?**

No

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**Session Classification:** Poster1

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