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Tranport properties of LiPF6 in PEO-PDMS polymer matrix

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Abstract content
   (Max 300 words)

Molecular dynamics simulations have been done to investigate the effect of PDMS side chain size and spacing on the diffusion of LiPF6 in PEO polymer matrix. The effect of temperature and concentration on LiPF6 diffusion in PEO-PDMS was also studied. Since Dreiding force field is not parametized for the LiPF6, it had to be edited so in can model the salt- salt and the salt- polymer interactions. The edited force field reproduce the structural parameters which compare well with literature. There is no clear evidence to suggest that side chain size and spacing has an effect on the Li+ diffusion in PEO-PDMS system. However a high diffusion of Li+ is observed for side chain length of 9 PDMS units.

Apply to be
 consider for a student
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no

Level for award
 (Hons, MSc,
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n/a

Main supervisor (name and email)
and his / her institution

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No

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