

SAIP2012



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Contribution ID : 322

Transport properties of LiPF₆ in PEO-PDMS polymer matrix

Tuesday 10 Jul 2012 at 17:30 (02h00')

Abstract :

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 parametrized 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.

Award :

no

Level :

n/a

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Paper :

No

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Session classification : Poster Session

Track classification : Track A - Division for Condensed Matter Physics and Materials

Type : Poster Presentation