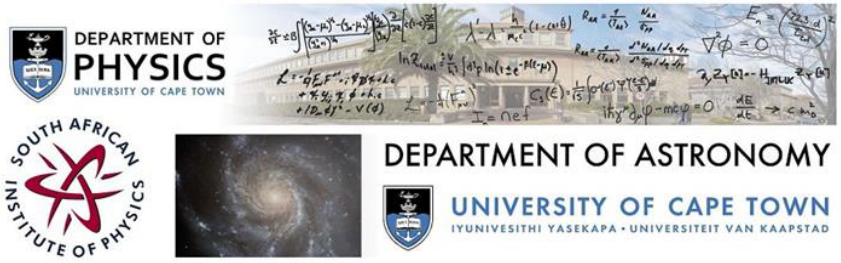

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Preparation of organically modified Vermiculite and calculation of intercalation energies of polymers into both unmodified and organically modified Vermiculite

Tuesday, 5 July 2016 16:10 (1h 50m)

Abstract content
   (Max 300 words)
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Computer modeling studies were performed to modify vermiculite with cetyl trimethyl ammonium bromide surfactant to form organically modified vermiculite and to investigate the intercalation energies of several polymers into unmodified vermiculite and organically modified vermiculite. Forcite module within Material Studio modelling interface was used to run the calculations. The force field employed in our studies is the universal force field. This force field has been found to be effective for most clay minerals. It was found that the intercalation energies of most polymers into unmodified vermiculite is higher than into organically modified vermiculite, which agrees with previous studies of vermiculite and polymer insertion into other 2:1 clays.

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PE Ngoepe phuti.ngoepe@ul.ac.za, Materials Modeling Centre, University of Limpopo, Sovenga, 0727, RSA

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Primary author: Mr PHALA, Michael Feredi (University of Limpopo)

Presenter: Mr PHALA, Michael Feredi (University of Limpopo)

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