Contribution ID: **137** Type: **Workshop**

Different Techniques of Force-field Derivation and Setting Up Molecular Dynamics (MD) Calculations at CHPC Using DL_POLY Code

Sunday, 1 December 2024 09:00 (1h 30m)

Molecular dynamics (MD) is a computer simulation method for studying the physical movements of atoms and molecules. The MD method can assist one in obtaining the static quantities and dynamic quantities. This method gives a route to dynamical properties of the system: transport coefficients, time-dependent responses to perturbations, rheological properties and spectra. The atoms and molecules are allowed to interact for a fixed period of time, giving a view of the dynamic evolution of the system. The DL_POLY Code parallel molecular dynamics simulation package will be utilised for exploration of such properties of molecular systems.

Student or Postdoc?

Email address

Co-Authors

CHPC User

CHPC Research Programme

Workshop Duration

Half-day

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