Proposal for a Workshop at 2024 CHPC National Meeting.

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

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Description:

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.

Duration: ½ day (3h)

Size: (max number of available seats)

Target Audience:

This one day workshop is intended for undergraduate project students, postgraduate students, postdoctoral researchers and researchers who are familiar with the field and want to employ state-of-the art methodology based on the density functional theory to understand bulk materials properties, surface science and heterogeneous catalysis phenomena.

Prerequisites: Familiarity with UNIX or Linux environment.

Type of Workshop: Mix of tutorials and hands-on (mostly practical)

Special requirements:

- Attendees need access to a laptop or workstation, active CHPC user account cluster with access to DL_POLY software.
- Open source spreadsheet such as Microsoft Excel with graphing capabilities is required for post-processing of output data.
- Free visualization softwares (e.g. VMD, VESTA, etc.), necessary for structure visualization.

- **Timetable: Please provide an outline of full syllabus**

Sunday (1 Dec 2024)

08:00	Registration
09:00	**Introduction to Molecular Dynamics** Properties of Molecular Dynamics Simulation code (DL_POLY) Fitting and validation of interatomic potentials Setting up molecular dynamic simulations
10:30	Morning Refreshment Break
11:00	**Force Field Models/ Interatomic Potentials** General Description Potential Models (Buckingham + Three-Body) Compatibility of Interatomic Potentials Validation
12:30	Lunch
13:30	**Hands-on exercises on:** Construction of Structure File Validation of Interatomic Potentials Generation of DL_POLY input files Submission of Calculations at CHPC Lengau
15:00	Afternoon Refreshment Break
15:30	
17:00	End of Day

- *For 90 minute workshop, only complete <u>one</u> session black; for a half-day workshop only fill in <u>two</u> session blocks. We cannot guarantee that your preferred session choice (morning or afternoon) will be available as we have to schedule the timetable according to available venues.*