Malaysia Branch

Monash University Malaysia

Webinar Talk on
"A Brief Introduction to Molecular Dynamics Simulations"

Jointly organized by The Institution of Mechanical Engineers (IMechE) Malaysia Branch and IMechE Monash University Malaysia Student Chapter

Date: 14 December 2021 (Tuesday)
Time: 2:00pm – 3.15pm (MYT)
Venue: Online Platform (Zoom)

Registration Fee
Fee: Free of charge

Synopsis
Molecular dynamics (MD) is a simulation approach to predict the physical motions of atoms. From the trajectories of atoms, we can learn about the thermodynamics of materials. The speaker's project has used MD to investigate the water permeation through porous graphene. Water and graphene were simulated as particles, and the liquid flow was simply the motion of these particles. The ability of MD simulations to study materials in nanoscale has made itself a potential tool in leading-edge research. This webinar will introduce the MD's working principles and a few simple examples, including the steps to perform MD through the open-source simulator, LAMMPS. The audiences can expect to acquire a brief understanding of MD and some ideas to start running the simulations from this webinar.

Speaker Profile
Mr Kueh Tze Cheng received his MEngSc by research from Multimedia University in 2016. He joined Monash University Malaysia in 2017 as a PhD student under the supervision of A/Prof. Hung Yew Mun, A/Prof. Kenny Tan, and Prof. Soh Ai Kah. His research focuses on water permeation through graphene nanostructures and molecular dynamics simulation.

Event Agenda

Activity	Time
Attendees Login	1.45 pm - 2.00 pm
Technical Talk	2.00 pm - 3.00 pm
Q&A Session	3.00 pm - 3.15 pm