Organised By :
WOMEN ENGINEERS SECTION, IEM

The Institution of Engineers, Malaysia

Physical Full-Day Workshop on Computational Chemistry for Engineering

This hands-on workshop introduces modern computational chemistry concepts, tools, and techniques to solve real-world engineering problems.

17th May 2025, Saturday
9.00 am - 5.00 pm

Auditorium Chin Fung Kee,
3rd Floor Wisma IEM, PJ

Speaker: ChM Dr. Erma Fatiha Binti Muhammad

an expert in computational chemistry with extensive experience in molecular modeling, cheminformatics, and materials engineering applications.

Who Should Attend?
Engineers, researchers, and students interested in computational chemistry applications

BEM Approved CPD Hours : 7
Ref No. : IEM25/HQ/133/W

REGISTRATION FEE'S (subject to 8% SST)		
	ONLINE FEE (Log-in for registration & payment: www.myiem.org.my/member/login.aspx)	**NORMAL FEE** (By Email : Payment by cash, credit card, bank-in, Quotation & Invoice)
IEM Student Members	100.00	150.00
IEM Graduate Members	200.00	250.00
IEM Corporate Members	400.00	450.00
Non-IEM Members	800.00	900.00

Website
www.myiem.org.my

SPEAKER : CHM DR. ERMA FATIHA BINTI MUHAMMAD

ChM Dr. Erma Fatiha Binti Muhammad is an expert in computational chemistry with extensive experience in molecular modeling, cheminformatics, and materials engineering applications. She has contributed to various research projects involving quantum mechanics, molecular dynamics simulations, and machine learning applications in chemistry.
With a strong academic background and practical expertise, Dr. Erma has trained researchers and industry professionals in computational chemistry techniques. Her passion lies in bridging theoretical chemistry with real-world engineering challenges, making her an inspiring speaker for this workshop.

SYNOPSIS

This hands-on workshop provides a comprehensive introduction to computational chemistry, focusing on its applications in engineering. It is structured into two key parts:

Basic Principles of Computational Chemistry
Participants will explore fundamental concepts, including:

- Molecular Mechanics & Force Fields – Understanding energy optimization and molecular interactions.
- Molecular Dynamics (MD) – Simulating molecular behavior using Newton's equations of motion.
- Electronic Structure Theory – Applying quantum mechanics to chemical systems.
- Cheminformatics – Using computational tools to analyze chemical structures and reactions.
- Machine Learning in Computational Chemistry – Implementing AI techniques for material discovery.

Basic Programming & Hands-on Activities
Attendees will gain practical experience by:

- Setting up and running molecular simulations using GROMACS.
- Visualizing molecular structures with Material Studio, Blender, and PyMOL.
- Performing QSAR analysis for material engineering with RDKit.
- Developing a Python virtual environment for computational chemistry projects.

This workshop equips participants with essential skills and hands-on experience in computational chemistry, bridging theory with real-world applications in engineering and material sciences.

PROGRAMME

Time	Programme
8.30 am to 9.00 am	Registration & Breakfast
9.00 am to 9.10 am	Opening Remarks by IEM-WE chairlady
9:10 am to 1.00 pm	**Part A: Basic Principles of Computational Chemistry for Engineering**
1.00 pm to 2.00 pm	Lunch break
2.00 pm to 5.00 pm	**Part B: Basic Programming in Computational Chemistry for Engineering with Hands-on Activity**
5.00 pm to 5.10 pm	Closing Speech
5.10 pm to 5.30 pm	Tea Break & Networking