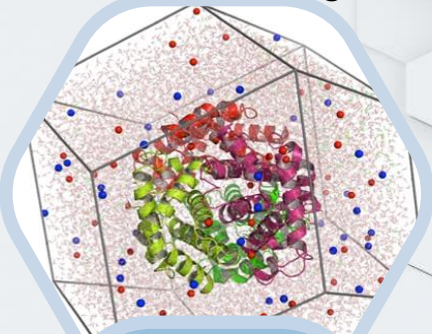




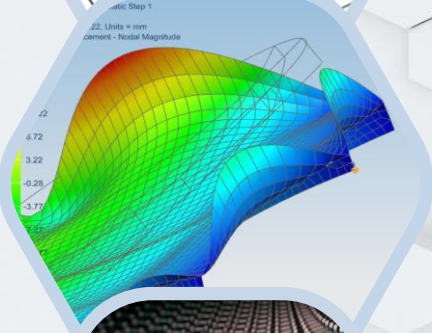
2022 School on Computational Physics modeling

19th December – 24th December
2022


Mohammed VI Polytechnic University
Benguerir



The Institute of Applied Physics (**IAP**) is pleased to host the **2022 School on Computational Physics**. Lectures, Teamwork, and Mentoring are part of the school to help you learn about computational physics and enhance your career.



Day 1 & 2:- Welcome / Introduction to Density Functional Theory (DFT) and Quantum simulation / Applications of ***DFT Simulation*** of the electronic structure of materials.



Day 3 & 4 : Introduction to ***Monte Carlo Simulation*** for Particles interactions and Materials Science Applications.

Day 5 & 6: Introduction to ***Molecular Dynamics*** / Hands-on session on LAMMPS Software.

Registration Fees

Academic: 2500 Dhs / Industrial: 5000 Dhs

The fees cover restaurant and accomodation in campus for the school period

Computational Physics School

Program: *Density Functional Theory*

Monday, 19 December 2022

08:30 – 9h00

Coffee Break

09:00 - 10 :30

Lecture 1: Introduction to DFT 1

10:30 – 12H

Lecture 2: Introduction to DFT 2

12:00-14 :00

Lunch break

14:00-15 :30

TP 1: Initiation to Quantum Espresso

15:30-17 :00

TP 2: Structure creation / Quantum Espresso input

18:30-19:30

Night Seminar: Theoretical investigations of electronic, optical, and thermoelectric properties of perovskite materials

Tuesday, 20 December 2022

08:30 – 9h00

Coffee Break

09:00-10 :30

TP 3: Relaxation / Self and non-self consistency

10:30-12 :00

TP 4: Density of states / Bandstructure

12:00-14 :00

Lunch break

14:00-15 :30

Projects assignment 1

15:30-17 :00

Projects assignment 2

18:30-19 :30

Night Seminar: Structural, electronic, magnetic and magnetocaloric; properties in metallic antiperovskites

Computational Physics School

Program: *Monte Carlo Simulation*

Wednesday, 21 December 2022

08:30 - 9h00

Coffee Break

09:00 - 10 :30

Lecture 1: Geant4, introduction and Geometry

10:30 - 12 :00

Lecture 2: Generation of primary particles

12:00 - 14 :00

Lunch break

14:00 - 15 :30

Lecture 3: physics lists

15:30 - 17 :00

TP 1: Geant4

18:30 - 19 :30

NIGHT SEMINAR: Monte Carlo Simulation for medical imaging

Thursday, 22 December 2022:

08:30 - 9h00

Coffee Break

09:00 - 10 :30

Lecture 4: introduction to Root

10:30 - 14 :00

TP 2: GATE application in medical imaging

12:00 - 14 :00

Lunch break

14:00 - 15 :30

TP 3: GATE/Root for data analysis

15:30 - 17 :00

TP 4: GATE/Root for data analysis

18:30 - 19 :30

Night Seminar: Calibration of the Detector ATLAS using Monte Carlo Simulation

Computational Physics School

Program: *Molecular Dynamics Simulation*

Friday, 23 December 2022:

08:30 - 9h00

Coffee Break

09:00 - 10 :30

Lecture 1: Introduction to Molecular Dynamics 1

10:30 - 12 :00

Lecture 2: Introduction to Molecular Dynamics 2

12:00 - 14 :00

Lunch break

14:00 - 15 :30

TP 1: Application to Ionic Liquids: Environment Preparation 1

15:00 - 17 :00

TP 2: Application to Ionic Liquids: Environment Preparation 2

18:30 - 19 :30

NIGHT Seminar: Exfoliation and re-aggregation mechanisms of black phosphorus: A molecular dynamics study

Saturday, 24 December 2022:

08:30 – 9h00

Coffee Break

09:00 - 10 :30

TP 3: Application to Ionic Liquids: Environment Preparation 3

10:30 - 12 :00

TP 4: Application to Ionic Liquids: Environment Preparation 4

12:00 - 14 :00

Lunch break

14:00 - 15 :30

TP 5: Application to ionic liquids: Results and discussions 1

15:30 - 17 :00

TP 6: Application to ionic liquids: Results and discussions 2

19:30

IAP End of Year DINNER