QUANTUM SIMULATIONS TECHNIQUES;

HiLAPW

It is designed to perform band-structure calculations based on the density functional theory (DFT). Its main features include scalarrelativistic spin-polarized calculations within the local (spin) density approximation (LSDA); all-electron self-consistent calculations; total-energy and atomic-force calculations for determining the equilibrium structure and phonons; electron density-of-states (DOS) calculations; and electron density and potential function calculations for 2D or 3D drawings.

STATE-Senri

It is a first-principles molecular dynamics code based on density functional theory (DFT) using a plane wave basis set and ultrasoft pseudopotentials. STATE was designed to perform band structure, total energy and molecular dynamics calculations on parallel supercomputers. The main features include are Norm-conserving pseudopotentials, LSDA & PBE, LDA+U, Iterative diagonalization , Automatic K-points generation , and etc.

MACHIKANEYAMA (KKR)

It used for first-principles calculation of electronic structures of metals, semiconductors and compounds, in the framework of the local density approximation or generalized gradient approximation (LDA/GGA) of the density functional theory. It is an all-electron method. It does not suffer from any serious truncation errors such as those of the plane-wave cutoff. Moreover AkaiKKR is combined with CPA (coherent potential approximation). Thus it is suitable not only for normal ordered crystals but also for disordered systems such as impurity systems, random substitutional alloys and mixed crystals. Since the method directly calculates the Green's function of the system, it can also provide a good starting point for first-principles linear response theory, many-body theory, and so on.

Wednesday 27 July 2022 (Day 1)	
Time (Kuala Lumpur GMT+8)	**Activities**
9.00am – 12.00pm	**Welcoming Remarks** Prof. Dr. H'ng Paik San (Head of Biopolymer and Derivatives Laboratory, INTROP)
	Sharing Session 1: Introduction to Computional Material Design, CMD and Introduction to DFT Prof. Dr. Tamio Oguchi (Osaka University, Japan)
	Sharing Session 2: Introduction to Linux system Dr. Mohd Farid Ismail (Faculty of Science, UPM)
	Q&A Session
	END OF SESSION FOR DAY 1
Thursday (28 July 2022) (Day 2)	
Time (Kuala Lumpur GMT+8)	**Activities**
9.00am – 12.00pm	**Sharing Session 3: Introduction to Machikaneyama (KKR)** Prof. Dr. Kazunori Sato
	BREAK
	Hands-on Session 1: Machikaneyama (KKR)
	Interpretation and Discussion Session 1: Machikaneyama (KKR) **- Case Study**
	END OF SESSION FOR DAY 2
Friday (29 July 2022) (Day 3)	
Time (Kuala Lumpur GMT+8)	**Activities**
9.00am – 12.00pm	**Sharing Session 4: Introduction to HiLAPW** Prof. Dr. Tamio Oguchi
	BREAK
	Hands-on Session 2: HiLAPW (Beginner level)
	Interpretation and Discussion Session 2: HiLAPW **- Case Study**
	END OF SESSION FOR DAY 3
Saturday (30 July 2022) (Day 4)	
Time (Kuala Lumpur GMT+8)	**Activities**
9.00am – 12.00pm	**Sharing Session 5: Introduction to STATE-Senri** Prof. Dr. Yoshitada Morikawa
	BREAK
	Hands-on Session 3: STATE-Senri
	Interpretation and Discussion Session 3: STATE-Senri **- Case Study**
	Closing Remarks Prof. Dr. Yoshitada Morikawa
	END OF PROGRAM

ASIACMD@UPM 2022
International Webinar on Computational Material Design
27 - 30 July 2022

ABOUT THE WORKSHOP

The virtual facilitated workshop is scheduled with Sharing, Hands-on and Discussion Sessions. The software installation instructions will be sent to the participant one week before the workshop. Participants are required to install the needed software (will be provided) before attending the workshop.

THE WORKSHOP INCLUDES

Upon completion of your registration for the workshop you will be sent

- A confirmation email which contains your access details to the virtual workshop held from 27 - 30 July 2022 .
- Software installation instructions.
- E-certificate of participation in workshop.

Registration Fees

RM200 for Malaysian participants
USD 55 for International participants
***Registration closes : Tuesday, 19 July 2022**

REGISTER NOW!

https://forms.gle/BYooojM3FMdcZ11A8

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