



1015 - 1045 Break

1045 - 1105 *"Graphitization and oxidative etching mechanism of the diamond surfaces studied by DFT and Graph Neural Network MD"*
Mr. John Isaac Enriquez, Osaka University

1105 - 1125 *"First-principles calculations of the electronic and optical properties of Cu-doped MoS₂"*
Ms. Melsa Rose Ducut, De La Salle University

1125 - 1145 *"Interplay of Hydrogen Boride Sheets with Water: Insights into Surface and Edge Stability"*
Mr. Kurt Irvin Rojas, Osaka University

1145 - 1200 Open Discussion (Question and Answer)

1200 – 1300 Lunch

Hands on Tutorials (Limited Slots)

1300 – 1700 Tutorial: *HiLAPW*
Prof. Tamio Oguchi, Osaka University

October 19, 2023

0800 – 1200 Tutorial: *STATE-Senri*
Prof. Yoshitada Morikawa, Osaka University

1200 – 1300 Lunch

1300 – 1700 Tutorial: *Machikaneyama*
Prof. Kazunori Sato, Osaka University

1700 Awarding of Certificates

Closing Remarks

Prof. Maria Cecilia Galvez
Chairperson
Department of Physics
De La Salle University

PART 2: