

14th Asia Computational Materials Design Workshop - 2022

Nov. 09	Nov. 10	Nov. 11	Nov. 12
<p>08:00-08:30: Registration</p> <p>08:30-09:00: Welcome Address and Introduction to PHENIKAA University, Prof. Nguyen Phu Khanh</p> <p>09:00-09:45: Invitation to Study in Osaka University, Prof. Tomoyuki Terai</p>	<p>08:30-09:10: Defect Interactions: Atomistic and Continuous, Prof. Yoji Shibutani</p> <p>09:10-09:50: Designing materials for energy applications: from defect physics to defect engineering, Prof. Hoang Khang</p>	<p>08:30-9:30: Lecture for HiLAPW, Prof. Tamio Oguchi</p>	<p>08:30-09:10: Valleytronics in 2D materials: Dispersion and flattening of band valleys and Exciton deformation under strain in WX₂ (X=S, Se), Prof. Dinh Van An</p> <p>09:10-09:50: Challenge of DFT to Glass Transition, Prof. Koun Shirai</p>
Break (15min)	Break (15min)	Break (15min)	Break (15min)
<p>10:00-11:00: Guidance for Use of PHENIKAA-HPC, Dr. Nguyen Viet Cuong</p> <p>11:00-12:00: Density Functional Theory for Electronic structures, Dr. Pham Tien Lam</p>	<p>10:05-11:05: Lecture for AkaiKKR, Prof. Kazunori Sato (OU)</p> <p>11:05-12:05: Hands-on Tutorial for AkaiKKR, Prof. Kazunori Sato</p>	<p>09:45-11:45: Hands-on Tutorial for HiLAPW, Prof. Tamio Oguchi</p>	<p>10:05-11:05: Lecture for STATE-senri, Prof. Ikutaro Hamada</p> <p>11:05-12:05: Hands-on Tutorial for STATE-senri, Prof. Ikutaro Hamada</p>
Lunch	Lunch	Lunch	Lunch
<p>13:30-15:30: Quantum ESPRESSO tutorial: Self-Consistent Calculations, Supercells, Structural Optimization, Dr. Nguyen Ngoc Linh</p>	<p>13:30-15:30: Hands-on Tutorial for AkaiKKR, Prof. Kazunori Sato</p>	<p>13:30-15:30: Hands-on Tutorial for HiLAPW, Prof. Tamio Oguchi</p>	<p>13:30-15:30: Hands-on Tutorial for STATE-senri, Prof. Ikutaro Hamada</p>
Break (15min)	Break (15min)	Break (15min)	Break (15min)
<p>15:45-16:45: Material database with IMMAD platform, Dr. Dang The Hung</p>	<p>15:45-16:45: Hands-on Tutorial for AkaiKKR, Prof. Kazunori Sato</p>	<p>15:45-16:25: Accelerating materials-science research via reproducible and open simulations with AiiDA, Materials Cloud and AiiDALab, Prof. Giovanni Pizzi</p>	<p>15:45-16:45: Hands-on Tutorial for STATE-senri, Prof. Ikutaro Hamada</p>
<p>16:45-17:00: Group picture & Break</p> <p>18:00-19:30: Welcome party</p>		<p>16:25-17:05: Atmospheric-Pressure Atomic Layer Deposition - An Avenue to Engineering Materials at the Atomic Level, Dr. Bui Van Hao</p>	<p>16:45-17:05: Certificate Conferring, Poster Prize and Closing Remarks</p>