

**WINTER SCHOOL ON
COMPUTATIONAL MATERIALS DESIGN
(CMD® Workshop, Vietnam), Can Tho University, December 06-09th, 2023**

Preliminary SCHEDULE

SR: Seminar Room (ATL), **Lab:** MoMa Lab (ATL), **HPC:** high performance computer; **ML:** machine learning; **AI:** artificial intelligence

December 06 (Lab)	December 07 (SR)	December 08 (Lab)	December 09 (Lab)
08:00-8:30, Registration for Hand-on HPC	08:00-8:30, Registration	08:00-09:00, Lecture 5 Prof. Yoshitada Morikawa, , Osaka Uni.	08:00-09:00, Lecture 6 Prof. Yoshitada Morikawa, Osaka Uni.
8:30-10:00 A/Prof. Nguyen Thanh Tien Linux and HPC	8:30-09:00, Opening remarks Rector of Can Tho Uni. Prof. Yoshitada Morikawa, Osaka Uni. 09:00-10:00: Short introduction in CMD, and Lecture 1: Prof. Tamio Oguchi, Osaka Univ. Group photo (10 mins)	09:00-10:00, (1h) Hands-on Tutorial 1 Prof. Tamio Oguchi, Osaka Univ.	09:00-10:00, (1h) Hands-on Tutorial 4 Prof. Yoshitada Morikawa, Osaka Uni.
Break (20 mins)	Break (20 mins)	Break (15 mins)	Break (15 mins)
10:20-11:20 A/Prof. Nguyen Thanh Tien, ML/AI in Computational Material	10:30-11:30, Lecture 2: Prof. Tamio Oguchi, Osaka Univ.	10:15-11:30, (1h15mins) Hands-on Tutorial 2 Prof. Kazunori Sato, Osaka Uni.	10:15-11:30, (1h15mins) Hands-on Tutorial 5 Prof. Kazunori Sato, Osaka Uni.
Free	Lunch	Lunch	Lunch
	13:30-14:30, Lecture 3 Prof. Kazunori Sato, Osaka Uni.	13:30- 15:30, (2h) Hands-on Tutorial 3 Prof. Tamio Oguchi, Osaka Univ.	13:30- 15:30, (2h) Hands-on Tutorial 6 Prof. Yoshitada Morikawa, Osaka Uni.
	Break (15 mins)	Break (15 mins)	Break (15 mins)
	15:00-16:00, Lecture 4 Prof. Kazunori Sato, Osaka Uni, 16:00-16:30, Presentation 1, Quantum molecular effects in nano scale devices (Dr. Deberati Dey Roy , Poddar Institute of Management & Technology, India)	15:45-16:15, Presentation 4, Ab initio prediction of anomalous Hall effect in antiferromagnetic CaCrO3 Dr. NGUYEN Thi Phuong Thao (Osaka Uni.) 16:15-16:45, Presentation 5, Recent achievement of first-principles studies for applications in solar cell devices (Dr. Triet , Can Tho Uni.)	15:45 – 16:15, Presentation 6, The title will be updated (Speaker) 16:15 – 16:45, Presentation 7, Feature-rich properties of emergent 1H-Na2S semiconducting monolayer: A hybrid functional study (Dr. Khanh , Van Lang Uni.)
	16:30-17:00, Presentation 2, Title: ??? Prof. Ikutaro Hamada (Osaka Uni.)	16:45, To visit the ecological garden	

	<p>17:00-17:30, Presentation 3, Elucidation of reaction mechanisms in NO_x purification catalysts using first-principle calculations. Dr. PHAM Ngoc Thanh (Osaka Uni.)</p>	<p>18:00, Welcome party</p>	<p>16:45-17:00, Certification of Completion Closing Remarks Prof. Yoshitada Morikawa, A/Prof. N. T. Tien</p>
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