

November 5-8, 2025: Hands-On Workshop at Shanghai University, East Campus

Time	Wednesday November 5, 2025	Thursday November 6, 2025	Friday November 7, 2025	Saturday November 8, 2025	Time	
09:00 - 10:00	09:00 - 10:00, Building 1, Room 101: Registration and Coffee	09:00 - 10:00, Building 1, Room 101: Yair Litman: <i>Ab Initio Molecular Dynamics</i>	09:00 - 10:00, Building 7, Room 510: Xinguo Ren: <i>Introduction to the GW Approximation for Excited States</i>	09:00 - 10:00, Building 7, Room 510: Yong Xu: <i>Challenges and Opportunities for Machine Learning of the Electronic Structure</i>	09:00 - 10:00	
10:00 - 11:00	10:00 - 10:30, <i>Introductory Remarks</i> : NOMAD Lab Director and Workshop Co-Organizer, Prof. Matthias Scheffler, Vice President of the SHU, Prof. Xuemei Yu, Vice Dean of the MGI of SHU, Prof. Jian Huang	10:00 - 10:30: Break	10:00 - 11:00, Building 7, Room 510: Lucas Foppa: <i>Big-Data Analytics and Machine Learning for Materials Science</i>	10:00 - 14:00, Building 7, Room 510: Hands-On Tutorial 4: <i>Artificial intelligence methods for materials science</i>	10:00 - 11:00	
	10:30 - 11:30, Building 1, Room 101: Xingao Gong: <i>Introduction to Electronic-Structure Theory and DFT</i>					10:30 - 11:30, Building 1, Room 101: Jiong Yang: <i>Introduction to Electron and Phonon Transport</i>
11:00 - 12:00	11:30 - 12:30, Building 1, Room 101: MS1P Team: <i>The Basics of FHI-aims</i>	11:30 - 12:30, Building 1, Room 101: Matthias Scheffler: <i>Modeling Heat and Charge Transport for Strongly Anharmonic Materials</i>	11:00 - 12:30, Building 7, Room 510: Break and Poster Discussions		11:00 - 12:00	
12:00 - 13:00	12:30 - 14:30, “Yixin” Canteen, 3rd floor: Lunch Break	12:30 - 14:30, “Yixin” Canteen, 3rd floor: Lunch Break	12:30 - 14:30, “Yixin” Canteen, 3rd floor: Lunch Break		14:00 - 15:00, “Yixin” Canteen, 3rd floor: Lunch Break	12:00 - 13:00
13:00 - 14:00						13:00 - 14:00
14:00 - 15:00				14:30 - 17:15, Building 7, Room 510: Hands-On Tutorial 1: <i>The Basics of Electronic Structure Theory</i>		14:30 - 18:15, Building 7, Room 510: Hands-On Tutorial 2: <i>Thermal and Electrical Transport Calculations</i>
15:00 - 16:00	Joint Farewell	15:00 - 16:00				
16:00 - 17:00		16:00 - 17:00				
17:00 - 18:00		17:00 - 18:00				
18:00 - 19:00		18:00 - 19:00				
19:00 - 20:00	19:00 - 21:00, "Panxi" Bookstore: Digital Poster Party, Get-Together	18:30 - 20:00, “Yixin” Canteen, West Campus: Dinner	18:30 - 20:00, “Lehu” campus hotel, West Campus: Conference Dinner		19:00 - 20:00	