Symposium on Materials Theory, driven by Aphrodite, *Ab Initio* Computations, and Artificial Intelligence (AI^3-2024), Paphos, Cyprus

	Tuesday November 5, 2024	TIME	Wednesday November 6, 2024	TIME	Thursday November 7, 2024	TIME	Friday November 8, 2024	TIME	Saturday November 9, 2024
			Session 1: *Ab Initio* Computations		**Session 2:** Artificial intelligence		**Session 3:** Catalysis, Transport, and More		**Session 3:** Catalysis, Transport, and More
		09:00	**Volker Blum:** Accurate Computational Materials Science for Real-Word Materials - FHI-aims and its Software Ecosystem	09:00	**Yong Xu:** Deep-learning electronic structure method developments	09:00	**Sergey Levchenko:** Combining theory, experiment, and artificial intelligence for the design of energy conversion materials	09:00	**Mariana Rossi:** Nuclear and electronic properties of 2D materials and interfaces boosted by machine learning
		09:45	**Sebastian Kokott**	09:45	**Kisung Kang**	09:45	**Herzain Rivera**	09:45	**Marios Zacharias:** A bottom-up high-throughput approach to anharmonic electron-phonon coupling in polymorphous materials
		10:15	Break	10:15	Break	10:15	Break	10:30	Break
		10:30	**Andrei Sobolev**	10:30	**Mario Boley:** From Prediction to Action: Critical Role of Performance Estimation for Machine-Learning-Driven Materials Discovery	10:30	**Yuanyuan Zhou:** AI-accelerated replica-exchange grand-canonical method for surface science: the case study of ammonia synthesis	11:15	Departure
		11:00	**Konstantin Lion**						
		11:30	**James Green**	11:15	**Akhil Nair**	11:15	**Ray Miyazaki:** Approach to catalytic chemistry by Artificial Intelligence and *Ab-Initio* calculation		
		12:00	Lunch	11:45	Lunch	12:00	Lunch		
		14:30	**Xinguo Ren:** Low-scaling GW method towards large-scale systems based on numerical atomic orbitals	13:30	Excursion from 13:30 - 18:00	14:30	**Jingkai Quan**		
		15:15	**Min-Ye Zhang**			15:00	**Yi Yao**		
		15:45	**Evgeny Moerman**			15:30	Break		
		16:15	Break			15:45	**Shuo Zhao**		
		16:30	**Parrydeep Sachdeva**			16:15	**Qaem Hassenzada**		
		17:00	**Manoj Dey**			16:45	Break		
		17:30	Break						
		19:00	Dinner	19:00	Dinner	19:00	Dinner		
19:00	Arrival	21:00	**Stefano Curtarolo:** Disordered enthalpy–entropy descriptor for high-entropy ceramics discovery	20:00	**Alexandre Tkatchenko:** Fully Quantum-Mechanical Biomolecular Simulations: From Dream to Reality	21:00	**Aaron Kelly:** Quantum Quality with Classical Cost: *Ab Initio* Nonadiabatic Dynamics Simulations using the Mapping Approach to Surface Hopping		
21:00	Dinner			20:45	Panel Discussion				
22:00	Welcome and Introduction: **Matthias Scheffler**								