

CUI/AIM & MPSD Workshop “Polaritonics from first principles”

Monday 2 October 2023

Morning session (08:45 - 12:25)

time	[id] title	presenter
08:45	[4] Welcome	RUBIO, Angel PUPILLO, Guido RUGGENTHALER, Michael SCHWARTZ, Tal
09:00	[2] Exploring Electrical Conductance of Amorphous Non-conducting Polymers under Vibrational Strong Coupling	THOMAS, Anoop
09:40	[3] Analysis of cavity-suppressed reactivity via vibrational depopulation	SIMPKINS, Blake
10:20	Coffee break	
11:05	[5] Local vs. collective interplay of (thermal) fluctuations in polaritonic chemistry Submitting author	SIDLER, Dominik
11:45	[6] How do chemical bonds break in ultrastrong coupling?	HERRERA, Felipe

Tuesday 3 October 2023

Morning session (09:00 - 12:25)

time	[id] title	presenter
09:00	[11] Insight from first principles: Embedding Techniques, Rate and Thermodynamic Changes, Solvation Effects, and Chiral Polaritonics	SCHAEFER, Christian
09:40	[15] Beyond the cavity	BARNES, Bill
10:20	Coffee break	
11:05	[17] Ultrafast dynamics of molecular polaritons	XIONG, Wei
11:45	[14] Molecular cavity dynamics: Numerical experiments and theoretical interpretations	NITZAN, Abraham