TYC20 Programme of talks

Day 1 - Monday 14 December 2026

09:00 - 09:30	Registration, Tea/Coffee
09:30 - 09:35	Celebrations opened by TYC Management Team members
09:35 – 09:40	Welcome Address - Giovanna Tinetti, Vice Dean for Research, Faculty of Natural, Mathematical and Engineering Sciences, King's College London
09:40 - 09:50	Historical Perspective – Mike Finnis FRS, Chair in Materials Theory and Simulation, Imperial College London
09:50 - 10:00	Historical Perspective – Angelos Michaelides FRS, 1968 Professor of Chemistry, University of Cambridge

Session 1: Functional Materials. Chair: Martijn Zwijnenburg (UCL) / Jarvist Frost (Imperial)

10:00 - 10:30	Nicola Marzari, University of Cambridge: It was the best of times, it was the worst of times...
10:30 - 11:00	Giulia Galli, The University of Chicago Materials for quantum technologies: the virtue of defects
11:00 - 11:30	Coffee
11:30 - 12:00	Karsten Reuter, Fritz Haber Institut: Embrace the Mess: Towards the Modeling of Disordered Catalyst Surfaces
12:00 - 12:30	Rachel Crespo-Otero, University College London Embedded cluster calculations on organic solids and MOFs
12:30 - 14:00	Lunch

Session 2: Machine Learning. Chair: Alex Ganose (Imperial)

14:00 - 14:30	Klaus-Robert Mueller, TU Berlin AI for the Sciences - Toward understanding
14:30 - 15:00	Gabor Csanyi, University of Cambridge ML force fields: status and some challenges
15:00 - 15:30	Keith Butler, University College London Machine learning for materials science; a bittersweet lesson
15:30 - 16:00	Coffee

Session 3: Roadmapping session. Chair: Jochen Blumberger (UCL)

16:00 - 17:30	Roadmapping Session
17:30 - 18:30	Drinks reception
19:00 - 22:00	Conference Dinner: Olea Social, 10 Upper St Martin's Lane, WC2H 9FB

Day 2 - Tuesday 15 December 2026

08:30 - 09:00 Registration, Tea/Coffee

Session 4: Electronic Structure. Chair: Hugh Burton (UCL)

09:00 - 09:30	Lucia Reining, Ecole Polytechnique Design of functionals: needs, news and thoughts
09:30 - 10:00	Andreas Grüneis, TU Wien Status and Future Challenges for periodic Coupled-Cluster Simulations in Materials
10:00 - 10:30	Paola Gori-Giorgi, Microsoft Research Skala: A Deep-Learning Route to Predictive Density Functional Theory

10:30 - 11:00 Coffee

Session 5: Biomaterials. Chair: Edina Rosta (UCL)

11:00 - 11:30	
11:30 - 12:00	Andrea Cavalli, CECAM Genomics meets Artificial Intelligence to transform Drug Discovery for Precision Medicine
12:00 - 12:30	Dominique Hoogland, King's College London Atomistic insights in to drug-lipid interactions
12:30 - 13:00	Modesto Orozco, Institute for Research in Biomedicine Barcelona:

13:00 - 14:30 Lunch

Session 6: Perspectives on Materials Modelling. Chair: Carla Molteni (King's)

14:30 - 15:00	Michele Parrinello, Italian Institute of Technology The Material Science of Catalysis
15:00 - 15:30	Clotilde Cucinotta, University of Florida:
15:30 - 16:00	Alessandro Troisi, University of Liverpool Computations for Discovering New Functional Molecules and Polymers
16:00 - 16:30	Angelos Michaelides, University of Cambridge Accurate simulations of interfaces are not easy
16:30 - 16:40	Closing remarks