Molecular Mechanisms of Tribochemistry and Lubrication

January 27, 2020 to January 29, 2020
Location: CECAM-HQ-EPFL, Lausanne, Switzerland

Organizers

Lorenz Chris King's College London
Righi M. Clelia University of Modena and Reggio Emilia
Tysoe Eddy University of Wisconsin-Milwaukee

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Monday 27th January

9:00 – 9:15 Opening Remarks
Chairman: Jean Michel Martin

9:15 – 10:00 Keynote Lecture: Rob Carpick, University of Pennsylvania, USA
Tribochemical Reactions in Nanoscale Boundary Lubrication Studied in situ: Mechanisms and Applications

10:00 – 10:30 Invited Talk: Roland Bennewitz, University of Saarland, Germany
Force microscopy experiments on molecular mechanisms in lubrication

10:30 – 10:50 Contributed Talk: Eddy Tysoe, University of Wisconsin-Milwaukee
Probing and Understanding Elementary Steps in Tribochemical Reactions

10:50 – 11:20 Coffee Break
Chairman: Roland Bennewitz

11:20 – 11:50 Invited Talk: Jean Michel Martin, Ecole Centrale de Lyon, France
Liquid Superlubricity: A Hybrid Hydrogen bond Network Model

11:50 – 12:10 Contributed Talk: Bart Weber, University of Amsterdam and Advanced Research Center for Nanolithography, Netherlands
Fluorescence microscopy visualization of the roughness-induced transition between lubrication regimes

12:10 – 12:50 Round-Table: Real-Time Monitoring and Surface Analysis of Tribochemical Reactions.
Moderators: Eddy Tysoe and Rob Carpick

12:50 – 14:00 Lunch

Chairman: Seiji Kajita

14:00 – 14:45 Keynote Lecture: Martin Müser, University of Saarland, Germany
Effect of shear stress on chemical reactions in zinc-phosphate derivatives

14:45 – 15:15 Invited Talk: Michael Chandross, Sandia National Laboratory, USA
Tribochemistry of MoS₂ with Water and Oxygen
15:15 – 15:35 Contributed Talk: Gabriele Losi, University of Modena and Reggio Emilia
Ab initio molecular dynamics linked to Green’s functions for accurate multiscale simulation of friction and tribochemistry

15:35 – 16:05 Coffee Break
Chairman: Michael Chandross

16:05 – 16:35 Invited Talk: Seiji Kajita, Toyota Central R & D Labs, Japan
Computational design of high viscosity index oil by Monte-Carlo tree search and molecular dynamics simulations

16:35 – 17:05 Invited Talk: Markus Meuwly, University of Basel, Switzerland
Adhesion and Motion at and on Hydrated Surfaces

17:05 – 17:25 Contributed Talk: C. Heath Turner, The University of Alabama, Tuscaloosa, AL, USA
Modeling the kinetics and thermodynamics of tribofilm formation using atomistic kinetic Monte Carlo simulations

17:25 – 18:05 Round-Table: Molecular Dynamics and First Principles Calculations of Tribochemistry; Bridging Time and Length Scales. Moderators: Clelia Righi and Martin Müser

18:05 – 19: Welcoming Drinks

Tuesday 28th January
Chairman: Markus Meuwly

9:00 – 9:45 Keynote Lecture: Daniele Dini, Imperial College London, United Kingdom
Modelling the interplay between lubricants, surfactants and surfaces in tribological interactions: from density functional theory to molecular dynamics and beyond

9:45 – 10:15 Invited Talk: Sophie Loehlé, Total SA, France
Multi-scale modeling approach for friction modifiers of today and tomorrow: an industrial point of view

10:15 – 10:35 Contributed Talk: Stefan Peeters, University of Modena and Reggio Emilia
The tribochemistry of MoDTC additives by QM/MM and first principles simulations

10:35 – 11:05 Coffee Break
Chairman: Sophie Loehlé

11:05 – 11:50 Keynote Lecture: Ali Erdemir, Argonne National Laboratory, USA
Achieving Ultralow Friction and Wear on Coated Surfaces by Catalyst-driven Tribochemistry

11:50 – 12:10 Contributed Talk: James Ewen, Imperial College London, UK
Mechanochemical Decomposition of Phosphate Esters Confined and Sheared between Iron Oxide Surfaces


12:50 – 14:00 Lunch
Chairman: Tomas Polcar
14:00 – 14:45 Keynote Lecture: Jean-Francois Molinari, EPFL Lausanne, Switzerland
Modeling adhesive wear across scales
14:45 – 15:15 Invited Talk: Nic Spencer, ETH Zurich
Friction on Brushy Gels
Insights into the tribo-chemistry of lubricated tungsten/diamond sliding contacts
15:35 – 16:05 Coffee Break
Chairman: Nic Spencer
16:05 – 16:35 Invited Talk: Michael Moseler, Fraunhofer IWM, Germany
Atomistic Insights Into Lubricated Diamond Sliding Contacts
16:35 – 17:05 Invited Talk: Filippo Mangolini, UT Austin
Imaging X-Ray Absorption Spectroscopic Investigation of the Mechanisms behind the Environmental Dependence of the Tribological Properties of Amorphous Carbon Surfaces
17:05 – 17:25 Contributed Talk: Manuel Cobián, LTDS, Ecole Centrale Lyon, France
Effects of intercalated water on MoS$_2$ lubricity: a classical MD investigation
17:25 – 18:05 Round-Table: Tribocorner of Coatings. Moderators: Filippo Mangolini and Michael Moseler
19:30 – 22:00 Social Dinner

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Wednesday 29th January
Chairman: Oguz Gulseren
9:00 – 9:45 Keynote Lecture: Oded Hod, Tel Aviv University, Israel
Modeling Interlayer Interactions in Layered Materials: Theory and Applications to Tribology
9:45 – 10:15 Invited Talk: Thilo Glatzel, University of Basel, Switzerland
Single molecule adsorption an manipulation processes studied by scanning probe microscopy
10:15 – 10:35 Contributed Talk: Martina Stella, Imperial College, London, UK
Effects of intercalated water on MoS$_2$ lubricity: a classical MD investigation
10:35 – 11:05 Coffee Break
Chairman: Paolo Nicolini and Thilo Glatzel
11:05 – 11:35 Invited Talk: Oguz Gulseren, Bilkent University
An Electronic Structure Perspective of Sliding of 2D materials
11:35 – 12:05 Invited Talk: Tomas Polcar, University of Southampton, UK, and Czech Technical University, Czech Republic
Results of International Training Network project on 2D solid lubricants
12:05 – 12:35 Invited Talk: David Burris, University of Delaware, USA
Cartilage and joint mechanics: New insights into the conditions of the buried interface.

12:35 – 12:55 Contributed Talk: Mauro Ferrario, University of Modena and Reggio Emilia
Insights into the effects of humidity on the lubricity of graphitic materials & High throughput screening of the cleavage and shear strengths of crystals

12:55 – 14:00 Lunch

Chairman: David Burris

14:00 – 14:30 Invited Talk: Paolo Nicolini, Czech Technical University, Czech Republic
Computational nanotribology in layered materials

14:30 – 14:50 Contributed Talk: Dimitrios Mathas, University of Southampton, United Kingdom
An evaluation of equilibrium Green-Kubo and nonequilibrium molecular dynamics for viscosity simulations of lubricants at different temperatures and pressures


15:30 – 15:45 Closing Remarks