

Saturday September 23, 2023 (2nd day)

SESSION VIII TRIBOCHEMISTRY AT COMPUTING ANALYSIS

Chair: M. Kubo & J. Fontaine

08:30 - 08:55 (25 min)

O-16 Mechanochemistry at the Nexus of Exascale Computing, Quantum Computing, and Artificial Intelligence

Aiichiro Nakano¹ (¹*University of Southern California*)

08:55 - 09:20 (25 min)

O-17 High-Throughput First-Principles Prediction of Interfacial Adhesion in Metal-on-Metal Contacts

M. Clelia Righi¹ (¹*University of Bologna, Italy*)

09:20 - 09:45 (25 min)

O-18 The Effect of Chemical Interactions on Dissipation Mechanisms in Condensed Matter: From Simple Alkanes via Ice to Bulk-Metallic Glasses

Martin H. Müser¹, Achraf Atila¹ and Hongyu Gao¹ (¹*Saarland University, Germany*)

< Tea Break (20 min) >

SESSION IX TRIBOCHEMISTRY IN MICA AND GRAPHITE

Chair: S. Glavatskih & Y. Meng

10:05 - 10:30 (25min)

O-19 On the Humidity Dependence of Highly Loaded Graphite Contacts

Martin Dienwiebel^{1,2}, Carina Morstein², Andreas Klemenz¹—and Michael Moseler^{1,3} (¹ *Fraunhofer-Institute for Mechanics of Materials IWM, German*
²*Karlsruhe Institute of Technology (KIT), IAM - Institute for Applied Materials,*

Germany, ³Institute of Physics, University of Freiburg, Germany)

10:30 - 10:55 (25 min)

O-20 Concentration Dependent Three Dimensional(3D) Hydration Structure in Non-Spherical ion Solution at Liquid-Solid Interface

Han Li¹, Zhi Xu¹, Ming Ma^{1*} (¹Tsinghua University, China)

SESSION X TRIBOCHEMISTRY IN MICA AND GRAPHITE

Chair: R. Crockett & H. Washizu

10:55 - 11:20 (25 min)

O-21 Formation of Intermittent Covalent Bonds at High Contact Pressure Limits Super-Low Friction on Epitaxial Graphene

Bartosz Szczefanowicz¹, Takuya Kuwahara^{2,3}, Tobin Filleter⁴, Andreas Klemenz², Leonhard Mayrhofer², Roland Bennewitz¹, Michael Moseler^{2,5} (¹Saarland University, Germany, ²Fraunhofer Institute for Mechanics of Materials IWM, Germany, ³Osaka Metropolitan University, Japan, ⁴University of Toronto, Canada, ⁵University of Freiburg, Germany)

11:20 - 11:45 (25 min)

O-22 Deep Neural Network Potential Applied for Tribocchemistry

Sophie LOEHLE¹, Alberto PACINI², Nam TRAN², Huong TA THI THUY², Paolo RESTUCCIA² and Maria Clelia RIGHI² (¹TotalEnergies, France, ²University Bologna, Italy)

11:45 - 11:55

COMMEMORATIVE PICTURE

11:55 - 13:00 (65 min.)

< Lunch >

POSTER SESSION

(13:00~15:00, 2 hours)

(Panel sizes: Width 0.9 m × Height 2.1 m)

Poster presentation is classified into the following two groups of A and B depending on the presentation time.

A Group (13:00 – 14:00 (1 hr.))

B Group (14:00 – 15:00 (1 hr.))

13:00 - 14:00 (1 hr.) **A Group**

P-01 Wear Analysis of Concentrated Polymer Brush via Coarse-Grained Molecular Dynamics simulations

Arisa Chiba¹, Ryutaro Kudo¹, Mizuho Yokoi¹, Masayuki Kawaura¹, Yuta Asano¹, Yusuke Ootani¹, Nobuki Ozawa^{2,1} and Momoji Kubo^{1,2}, (¹Tohoku University, Japan, ²Tohoku University, Japan)

14:00 - 15:00 (1 hr.) **B Group**

P-02 The Effect of Specimen Combinations on the Friction between Noble Metals and Ceramics

Jushiro TANAKA¹, Kenichi HIRATSUKA¹ (¹ Chiba Institute of Technology, Japan)

13:00 - 14:00 (1 hr.) **A Group**

P-03 Reactive Molecular Dynamics Simulation of Corrosion Wear at DLC/Fe Sliding Interface

Mizuho Yokoi¹, Masayuki Kawaura¹, Yuta Asano¹, Yusuke Ootani¹, Nobuki Ozawa^{2, 1}, Momoji Kubo^{1, 2} (¹ Institute for Materials Research, Tohoku University, Japan, ² New Industry Creation Hatchery Center, Tohoku University, Japan)

14:00 - 15:00 (1 hr.) **B Group**

P-04 Relationship between Solubility Parameter and molecular Structure of Viscosity Index Improvers in Various Base Oils

Sohei Nambo¹, Tomoko Hirayama¹, Nobuhiro Sato², Masaaki Sugiyama² and Yoriyuki Takashima³ (¹*Department of Mechanical Engineering and Science, Kyoto University, Japan*, ²*Institute for Integrated Radiation and Nuclear Science, Kyoto University, Japan*, ³*Idemitsu Kosan Co., Ltd, Japan*)

13:00 - 14:00 (1 hr.) **A Group**

P-05 An Open Boundary Condition of Molecular Dynamics Method for Realizing Continuous Tribochemical Reaction Simulations

Yuta Asano¹, Ryutaro Kudo¹, Arisa Chiba¹, Mizuho Yokoi¹, Masayuki Kawaura¹, Yusuke Ootani¹, Nobuki Ozawa^{2,1} and Momoji Kubo^{1,2} (¹*Institute for Materials Research, Tohoku University, Japan*, ²*New Industry Creation Hatchery Center, Tohoku University, Japan*)

14:00 - 15:00 (1 hr.) **B Group**

P-06 Photoelectron Emission from Real Copper Surfaces Adsorbed with Water, Alcohols, and Air

Yoshihiro Momose¹, Masakazu Honma¹ and Suguru Kohno¹ (¹*Ibaraki University, Japan*)

13:00 - 14:00 (1 hr.) **A Group**

P-07 Molecular Dynamics Simulation Analysis of Tribochemical Reaction and Friction Reduction Mechanism of Si₃N₄ in Water Lubrication with Ethylene Glycol

Ryutaro Kudo¹, Arisa Chiba¹, Mizuho Yokoi¹, Masayuki Kawaura¹, Yuta Asano¹, Yusuke Ootani¹, Nobuki Ozawa^{2,1} and Momoji Kubo^{1,2} (¹*Institute for Materials Research, Tohoku University, Japan*, ²*New Industry Creation Hatchery Center, Tohoku University, Japan*)

14:00 - 15:00 (1 hr.) **B Group**

P-08 Influence of Rolling Contact on the Sliding Wear of Aluminum

So Sato¹, Kenichi Hiratsuka¹ (¹*Chiba Institute of Technology, Japan*)

13:00 - 14:00 (1 hr.) [A Group](#)

P-09 Friction Behavior of Silicon Oxycarbide Coatings in Water

Tadashi Shiota¹, Kazuma Shimazaki¹, Ryosuke Ishi¹, Yuya Omiya² and Masahiro Fujii¹ (¹ Okayama University, Japan, ² Kagawa University, Japan)

14:00 - 15:00 (1 hr.) [B Group](#)

P-10 Study of Additive of MAC oil and Ionic Liquid as New Lubricants for Spacecraft

Takashi Yokoyama¹, Nobuo Kenmochi¹, Koji Matsumoto¹, Shingo Obara¹, Yusuke Nakanishi², Yukio Yoshida², Shizuka Agano³ (¹ Japan Aerospace Exploration Agency, Japan, ² Idemitsu Kosan Co., Ltd., Sodegaura, Japan, ³ Idemitsu Kosan Co., Ltd., Ichihara, Japan)

13:00 - 14:00 (1 hr.) [A Group](#)

P-11 Effect of Discharge Plasma on Electrical Properties of Aromatic Compounds

Satoshi Nouyama¹, Makoto Hayama¹, Daming Dong¹ and Keiji Nakayama² (¹ Kyodo Yushi Co. Ltd, Japan, ² Institute of Mesotechnology, Japan)

14:00 - 15:00 (1 hr.) [B Group](#)

P-12 Tribological Investigation of White Etching Cracks Based on a Tribometer-scale Approach

Hakim El Bahi¹, Christelle Vacher², Goulven Bouvier¹, Quentin Arnoux¹ (¹ TotalEnergies, France, ² NTN-SNR Roulements, France)

13:00 - 14:00 (1 hr.) [A Group](#)

P-13 Effect of Polymer Additives on Lubricant Flow in Narrow Gaps

Naoki Yamashita¹, Waka Yamamoto¹, Akira Okada¹ and Tomoko Hirayama¹ (¹ Kyoto University, Japan)

14:00 - 15:00 (1 hr.) [B Group](#)

P-14 Exploring the Influence of Grease Thickener on Lubrication Performance and Tribofilm Formation with ZDDP and MoDTC Additives

Akepati Bhaskar Reddy¹, Jeffrey James Black², Johan Leckner³, Jason B. Harper², Mark W. Rutland⁴ and Sergei Glavatskih¹ (¹ Department of Engineering

Design, KTH Royal Institute of Technology, Sweden, ²University of New South Wales, Australia, ³ Axel Christiernsson International AB, Sweden, ⁴Department of Chemistry, KTH Royal Institute of Technology, Sweden)

Announcement for “The Bus Tour – -Jigokumeguri - (The Hell Tour)”
Organizer: S. Nouyama & T. Maruyama

15:00 - 15:20 (20 min.)

<Break (20 min) >

15:20-17:30 (About 2 hrs.)

TOUR -Jigokumeguri-(The Hell Tour)

(Organizer: S. Nouyama & T. Maruyama)

15:20 Bus leaves at the Conference place (**B-Con Plaza**) for the Hell Tour.

17:30 Bus arrives at the Kamenoi Hotel.

< Break (30 min.)>

18:00-20:30 (2.5 hrs.)

BANQUET

<At the Kamenoi Hotel>

Chair: T. Shiota & S. Loehle

“AWARD CEREMONEY” will be held, where “The Tribochemistry Award” is presented to the following three scientists who made outstanding contributions to the science and technology in the field of tribochemistry.

• **Dr. Ali Erdemir**

Professor of Texas A&M University, U.S.A.

• **Dr. Antonella Rossi**

Professor of University of Cagliari, Italy

• **Dr. Nicholas D. Spencer**

Emeritus Professor of ETH Zurich, Switzerland.
