

UCSD NANOENGINEERING/CHEMICAL ENGINEERING
Virtual **SEMINAR SERIES**
Friday, July 15th, 2022
Seminar Presentation: 11:00am - 12:00pm PDT



“Ion and Electron Transfer at Solid-Solid Interface: DFT Calculation Study with Explicit Interface Model”

Dr. Yoshitaka TATEYAMA, PhD

*Group Leader of Interface Computational Science Group,
and Deputy Director of Center GREEN in
National Institute for Materials Science (NIMS), Tsukuba, JAPAN*

Abstract: Atomistic understanding of ion and electron transfer around "buried" solid-solid interface has been still an essential issue in various fields because of the difficulty of experimental as well as computational analyses. We have addressed DFT calculation studies of such interfacial reactions/phenomena in the battery and catalyst fields, via developing new techniques such as heterogeneous-interface CALYPSO method and utilizing high-performance computing such as the "Fugaku" supercomputer. In this talk, in addition to such methodology, I'll introduce our recent works on ion and electron transfer at electrode interfaces with sulfide and oxide electrolytes (e.g. Li, LiCoO₂ vs. LPS, LLZ, LATP) and LiCx/SEI interfaces. I'll also show the recent DFT-MD investigations of ion transport around "grain boundaries" with dopants in LLZ solid electrolyte. Finally, the common aspects in these works will be discussed. These works were mainly done in collaboration with Dr. B. Gao, Dr. H.-K. Tian and Dr. R. Jalem.

References: Chem. Mater. 32, 85 (2020); PCCP 22, 10764 (2020); ACS AMI 12, 16350 (2020); ACS AEM 3, 11061 (2020); ACS AMI 12, 54752 (2020); ACS AMI 13, 11765 (2021); JMCA 9, 15207 (2021); Adv. Energy Mater. 12, 2102151 (2022); ACS AEM 5, 98 (2022); JMCA 10, 10083 (2022).

Biosketch:

Education

1998: Ph. D.: Graduate School of Science, The University of Tokyo (Physics)
Supervisor: Prof. Shinji Tsuneyuki,

Professional experience

1998-2001 Researcher, National Research Institute for Metals
2001- National Institute for Materials Science (NIMS)
During this term, he had some visiting positions:
2003-2004 Visiting researcher in University of Cambridge
2007-2015 JST-PRESTO researcher
2016 Visiting researcher in Fritz Haber Institute of Max-Planck Society

Currently, Group Leader of Interface Computational Science Group, and Deputy Director of Center GREEN in NIMS.
2018--: Visiting Professor, Tokyo Institute of Technology
2018--: Visiting Professor, Waseda University

(Reference: https://www.nims.go.jp/group/cs/en/members/tateyama_e.html)