

高分子学会九州支部 外国人講演会

Chemical Processes at Surfaces and Interfaces. Insights from Theory

Associate Professor Aleksandar Staykov
Principle Investigator at the International Institute for Carbon Neutral Energy Research
Kyushu University, Japan

日時: 2020年12月4日(金) 11:00~12:00

場所: オンライン開催 (Webex を使用予定)

Abstract:

The lecture will cover modern computational approaches for investigation of surface and interface processes in materials and their practical applications for design of novel materials for catalysis and nanoelectronics. The orbital control of photochemical and electrochemical switching activity of diarylene molecules will be explained and it will be further expanded to the design of switchable oligomers such as diarylene capped sexithiophene wires (*ACS Nano* **2011**, *5*, 1165). The selective polymer wrapping on semiconducting CNTs will be introduced with formation of flavin-based helix-like supramolecular aggregates (*J. Am. Chem. Soc.* **2020**, *142*, 11847). The semiconducting CNTs selectivity will be further explored with the introduction of metal-organic complexes. Finally, the lecture will focus on the design principles for fabrication of nano-scale diodes based on selective doping in nano-carbon materials such as polycyclic aromatic hydrocarbons and graphene ribbons (*J. Phys. Chem. C* **2013**, *117*, 13644).

About the speaker:

2002: Mater degree in Organic Chemistry, Sofia University, Bulgaria

2006: PhD in Physical and Theoretical Chemistry, Leipzig University, Germany

2006-2008: Research associate Institute for Materials Chemistry and Engineering, Kyushu University, Japan

2008-2011: JSPS postdoctoral fellowship, Kyushu University, Japan

2011-2016: Assistant professor, International Institute for Carbon Neutral Energy Research, Kyushu University, Japan

2016-present: Associate professor and principle investigator, International Institute for Carbon Neutral Energy Research, Kyushu University, Japan

The laboratory of Dr. Staykov specializes in first-principle calculation of energy related materials and processes. Major research interests are catalysts for polymer electrolyte fuel cells, electrode surfaces in solid oxide fuel cells, electrolytes for lithium ion batteries, nanoparticle catalysis, nanoelectronics, structure and properties of carbon nanomaterials, and hydrogen embrittlement of metals. Dr. Staykov actively participates in the development of novel computational techniques for materials discovery based on machine learning and artificial intelligence in collaboration with the Institute for Mathematics in Industry, Kyushu University.

参加要領

- 1) 参加費: 無料、
- 2) 定員: 200名、
- 3) 申込方法: 氏名、所属、連絡先を明記の上、E-mailにてお申し込みください。
- 4) 申込締切 2020年12月3日(木)

申込・問い合わせ先

白木 智丈 (九州大学大学院工学研究院応用化学部門)

E-mail: shiraki@mail.cstm.kyushu-u.ac.jp、電話: 092-802-2841