

## Out of the Crystalline Comfort Zone: ML-Empowered Modelling of Operando Energy Conversion Systems

Prof. Dr. Karsten Reuter

(Director of the Theory Department,

Fritz-Haber-Institut der Max-Planck-Gesellschaft)



2023年9月11日(月) 11:00–12:00

(創成科学研究棟4階 セミナー室B・C)

<http://www.cat.hokudai.ac.jp/access.html>

Operando spectroscopies and microscopies reveal a highly dynamic behavior of interfaces in energy conversion systems. Predictive-quality modeling and simulation is presently essentially unable to address the substantial, complex and continuous morphological transitions at such working interfaces. I will review this context from the perspective of first-principles based multiscale modeling, highlighting that the fusion with modern machine learning approaches is key to tackle this complexity.

### [Academic Career]

- Director, Theory Department, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany, 2020–present
- Chair for Theoretical Chemistry & Catalysis Research Center, Technische Universität München, Germany Full Professor in Chemistry, Adjunct Professor in Physics, 2009–2020
- Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany Head of MPG Independent Junior Research Group “First-Principles Statistical Mechanics”, 2005–2009
- Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany Group Leader “Catalytic Reactions at Surfaces”, Theory Department, 2003–2005

### [Awards and Professional Recognition (selection)]

- Elected Henriette-Herz Scout, Alexander von Humboldt Society, 2021–present
- Visiting Professor, Dept. of Materials, Imperial College London, 2019–2020
- Lectureship of the Netherlands Center for Multiscale Catalytic Energy Conversion, 2019
- Visiting Professor, Dept. of Mechanical Engineering, MIT, U.S.A., 2018
- MPG Frontiers Award for Chemical Energy Conversion, 2018
- Visiting Professor, Dept. of Chemical Engineering, Stanford University, U.S.A., 2014–2015
- MPG Independent Junior Group Award, 2005

問合せ先: 触媒科学研究所・長谷川 淳也 教授 (hasegawa@cat.hokudai.ac.jp・011-706-9120)

共催: 触媒科学計測共同研究拠点, 学際統合物質科学研究機構