

# The Elucidation of Non-equilibrium States of Heterogenous Catalysis by Data-driven Multiscale Simulation: A Case Study of Methanol Synthesis

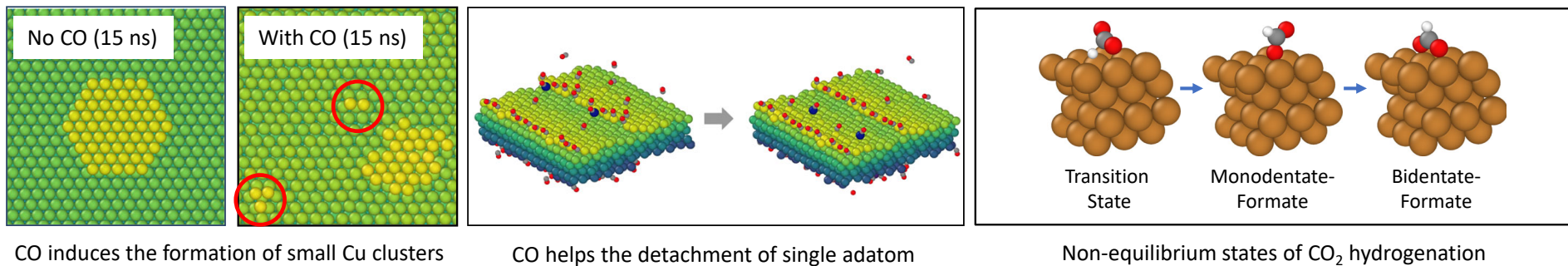
Graduate School of Engineering, Osaka University

Harry H. Halim, Ryo Ueda, Yuki Yamada

**Purpose** Elucidating non-equilibrium states of the interaction between  $\text{CO}_2$ ,  $\text{CO}$ , and  $\text{H}_2$  gases with Cu catalyst (i.e., early stage of methanol synthesis)

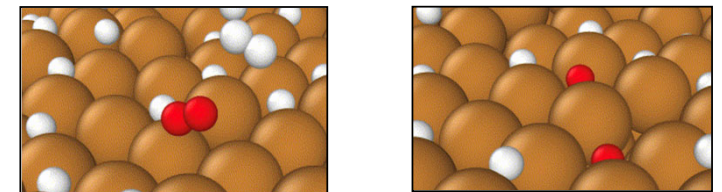
**Outline** Molecular Dynamics simulation driven by machine learning potential (MLP) is used to observe and measure atomistic events during non-equilibrium states. MLP is built based on first-principles data generated by active learning scheme.

## Result



Computing system:  
node-hour  
memory used  
parallelize

SQUID General Purpose CPU and GPU nodes  
55,920 node-hours (CPU), 2500 node-hours (GPU)  
1 TB  
1 node



Explicit splitting and recombination of  $\text{H}_2$  on Cu(111)