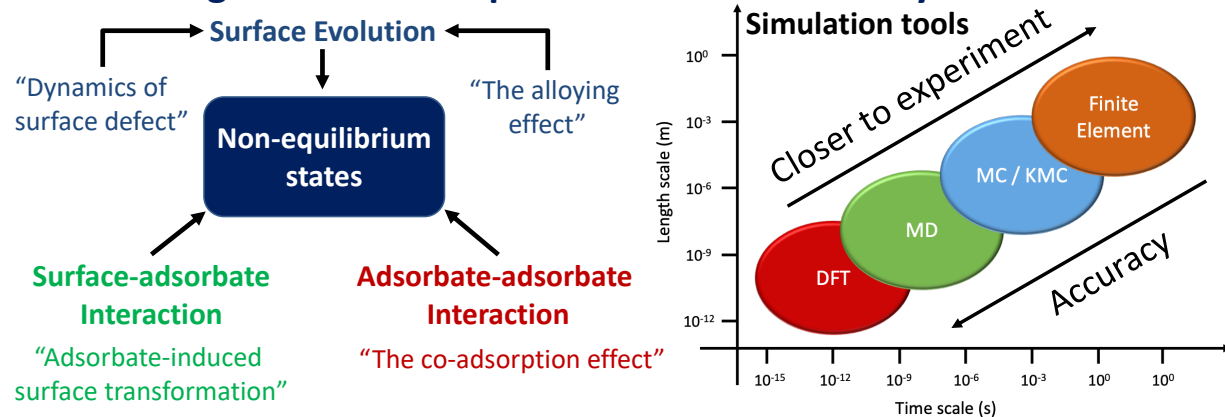


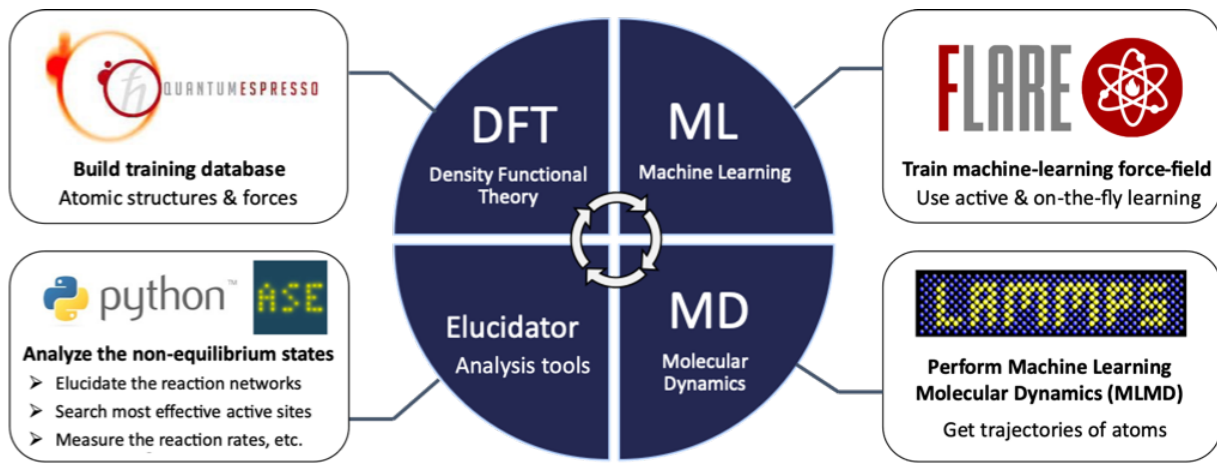
# Machine Learning-Driven Multi-Scale Simulations for Green Catalysis Design

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## The challenge of the non-equilibrium states of catalysis



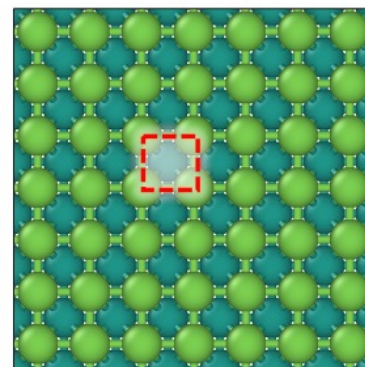
Objective: elucidate the behavior of catalysis at non-equilibrium states



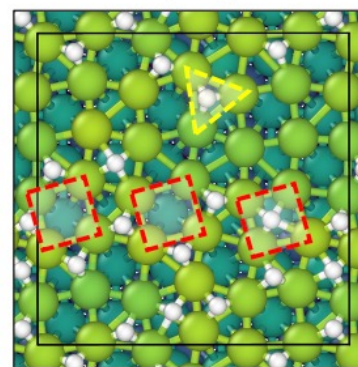
## #1 H-induced surface reconstruction on Cu(100) surface

*ACS Catalysis*, 2026, 16, 5, 5068–5079.

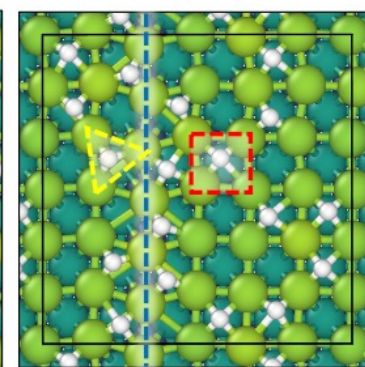
Pristine Cu(100) Surface



The R-Cu(100) Surface



The LS-Cu(100) Surface



## #2 CO-induced Cu clusters enhance WGS reaction

*Phys. Chem. Chem. Phys.*, 2026, (Advance Article).

