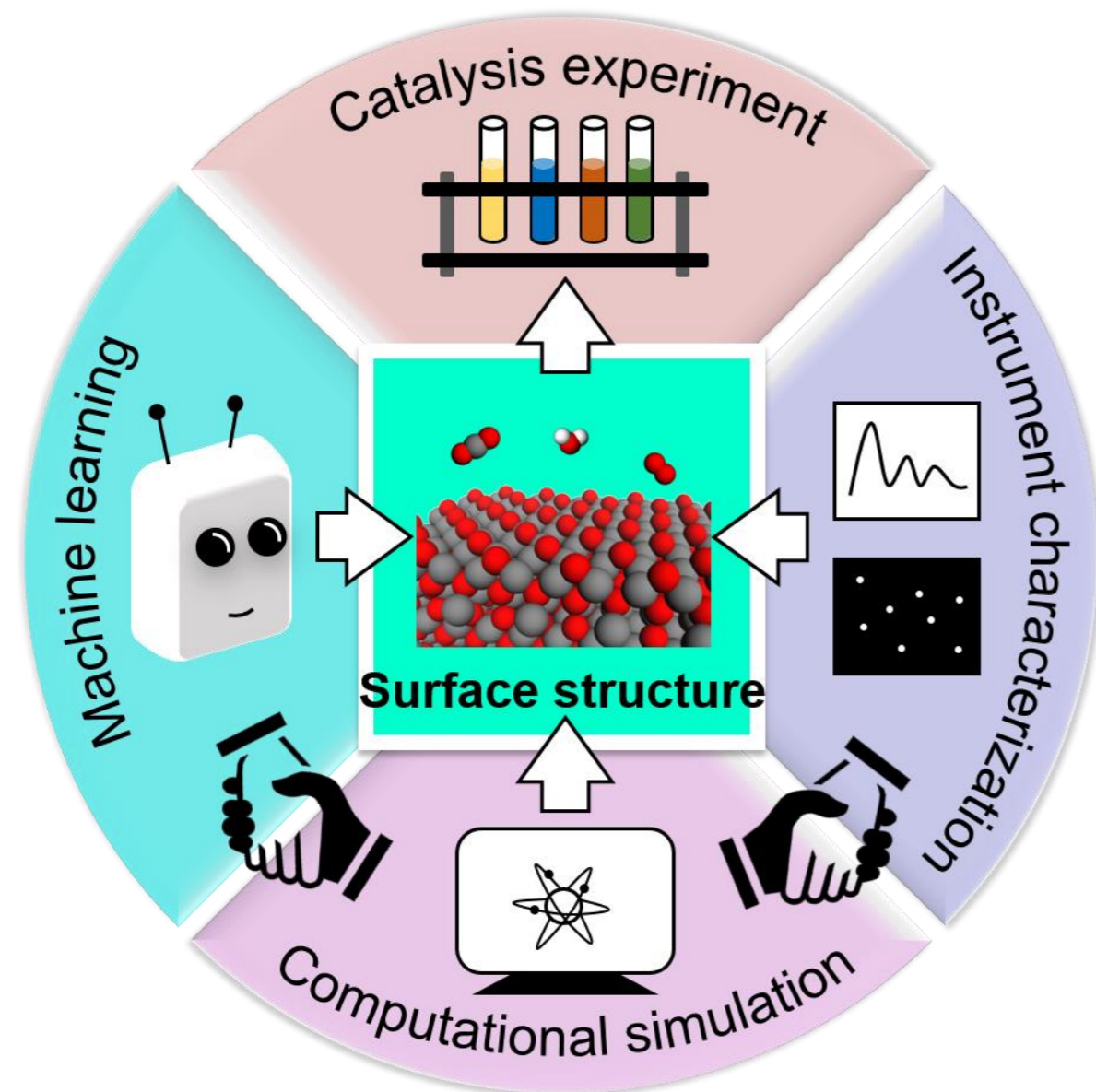


# AI-Driven *in-situ* Experimental Spectroscopy Analysis



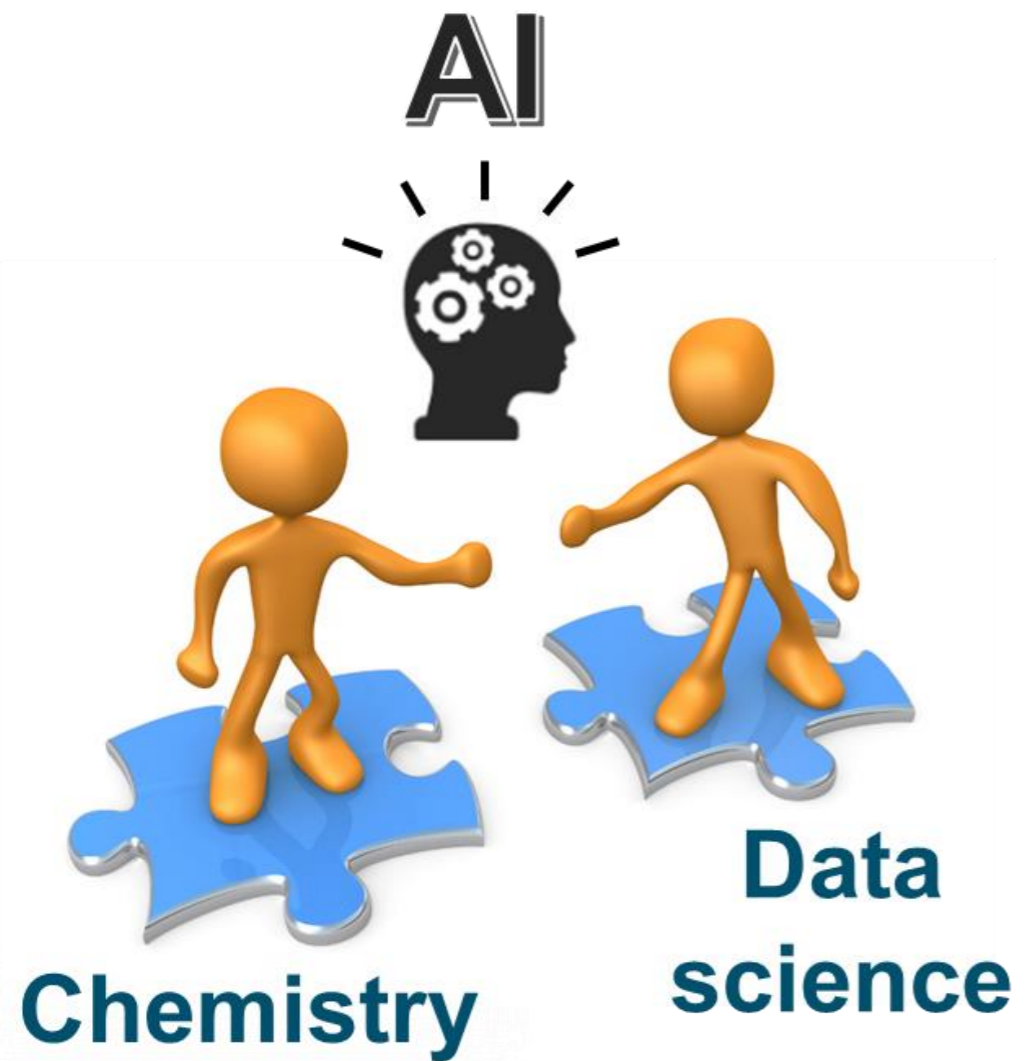
Haobo Li

Australian Research Council DECRA Fellow

The University of Adelaide, Australia

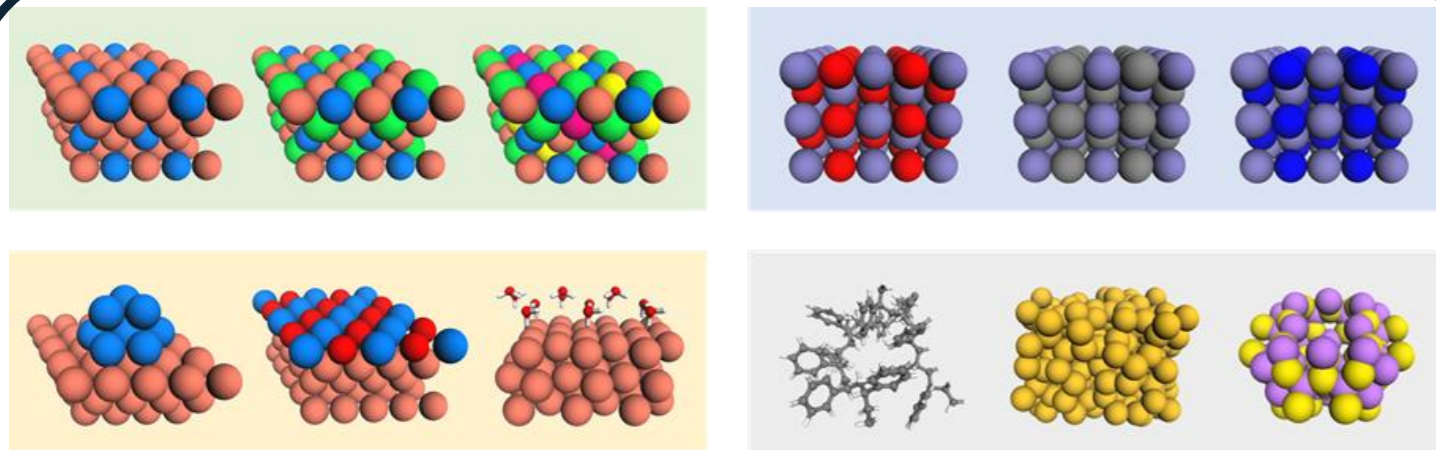
18/03/2024

# AI-driven energy catalysis: A rapidly emerging direction



*In chemistry, emerging AI unleashes its power to solve complex challenges and unearth novel insights.*

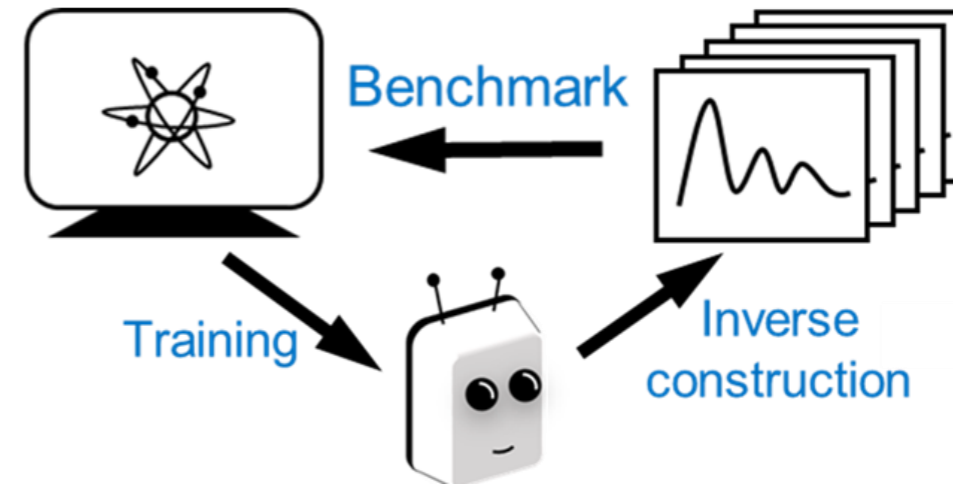
# AI applications: What can we do now?



Materials design

Surface structure

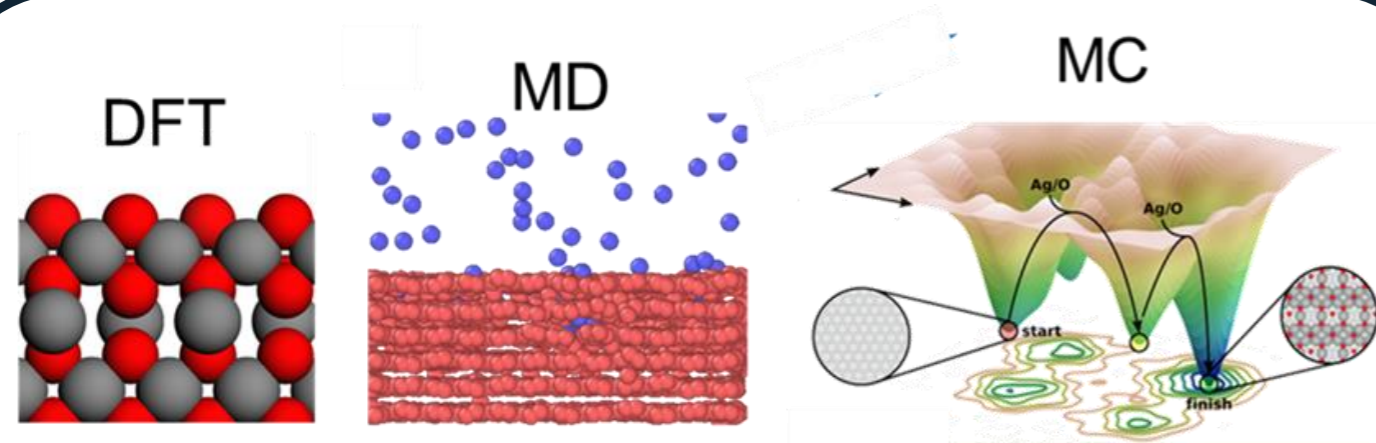
ACS Catal. 2021  
JACS 2023  
EES 2023



Experimental data mining

Reaction conditions

JPCL 2023



Multi-scale modelling

Reaction mechanism

Angew 2023



Very intuitive platform, I'll definitely recommend it. The chat support is excellent, really fast in their replies and very helpful.

Usability

Positive

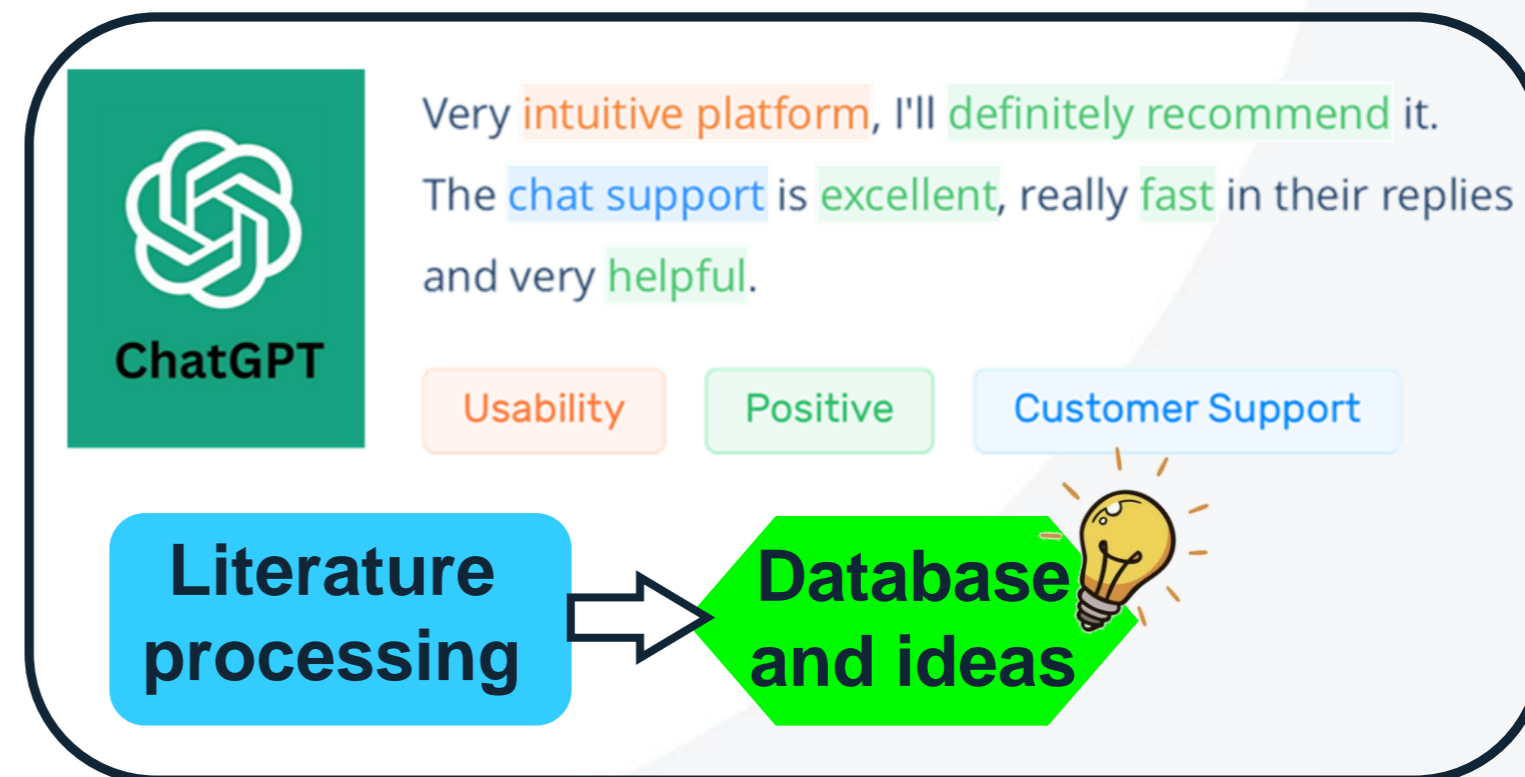
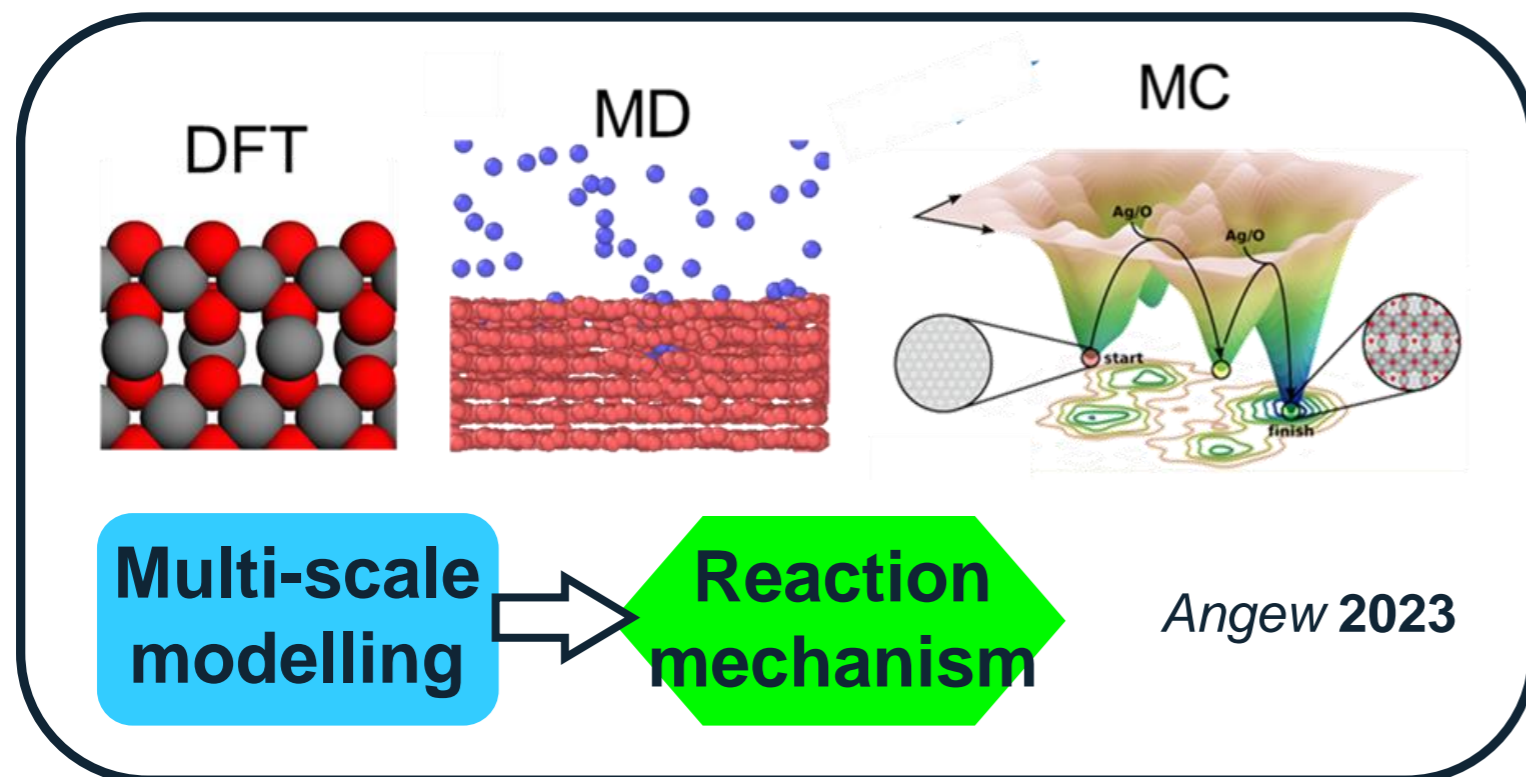
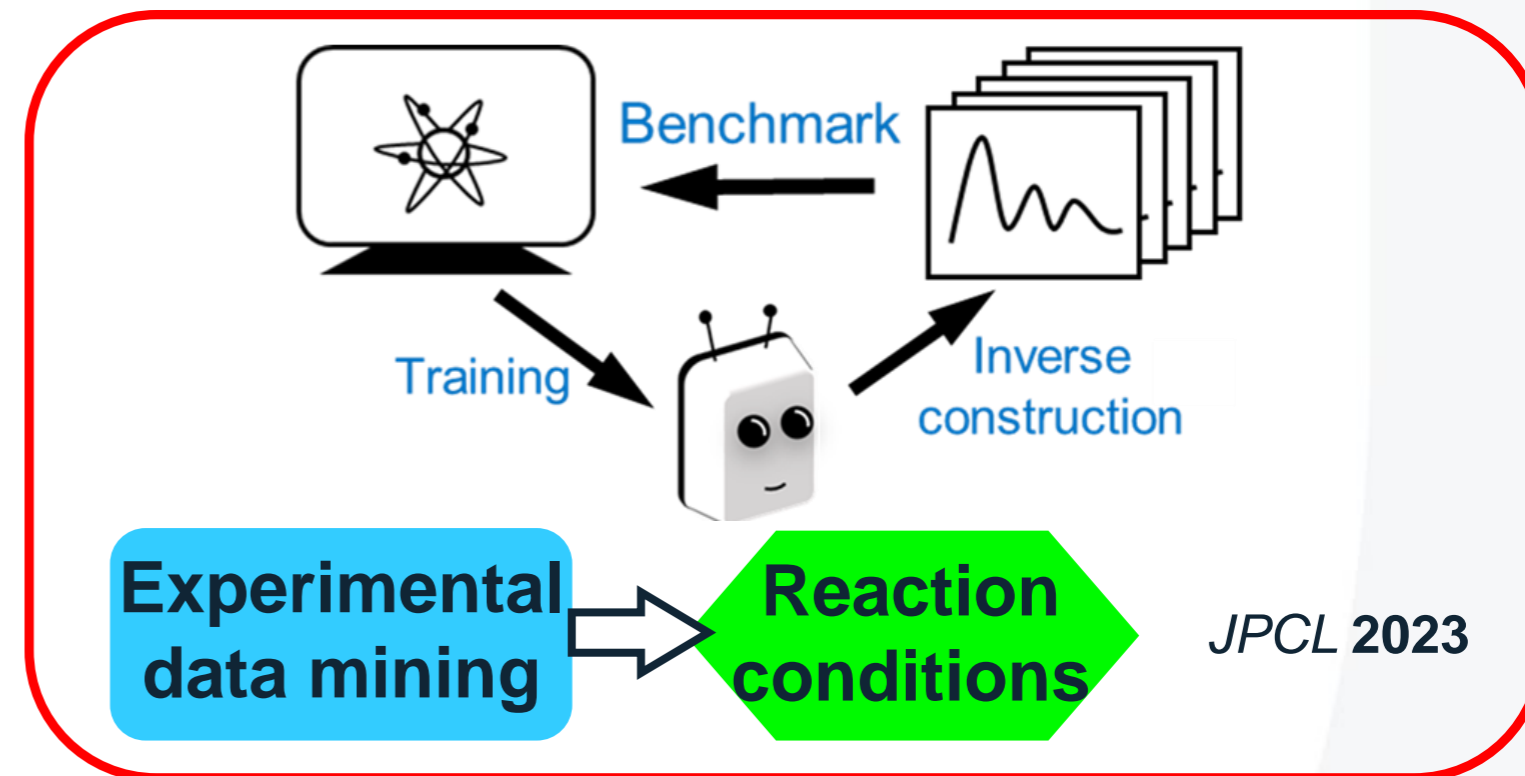
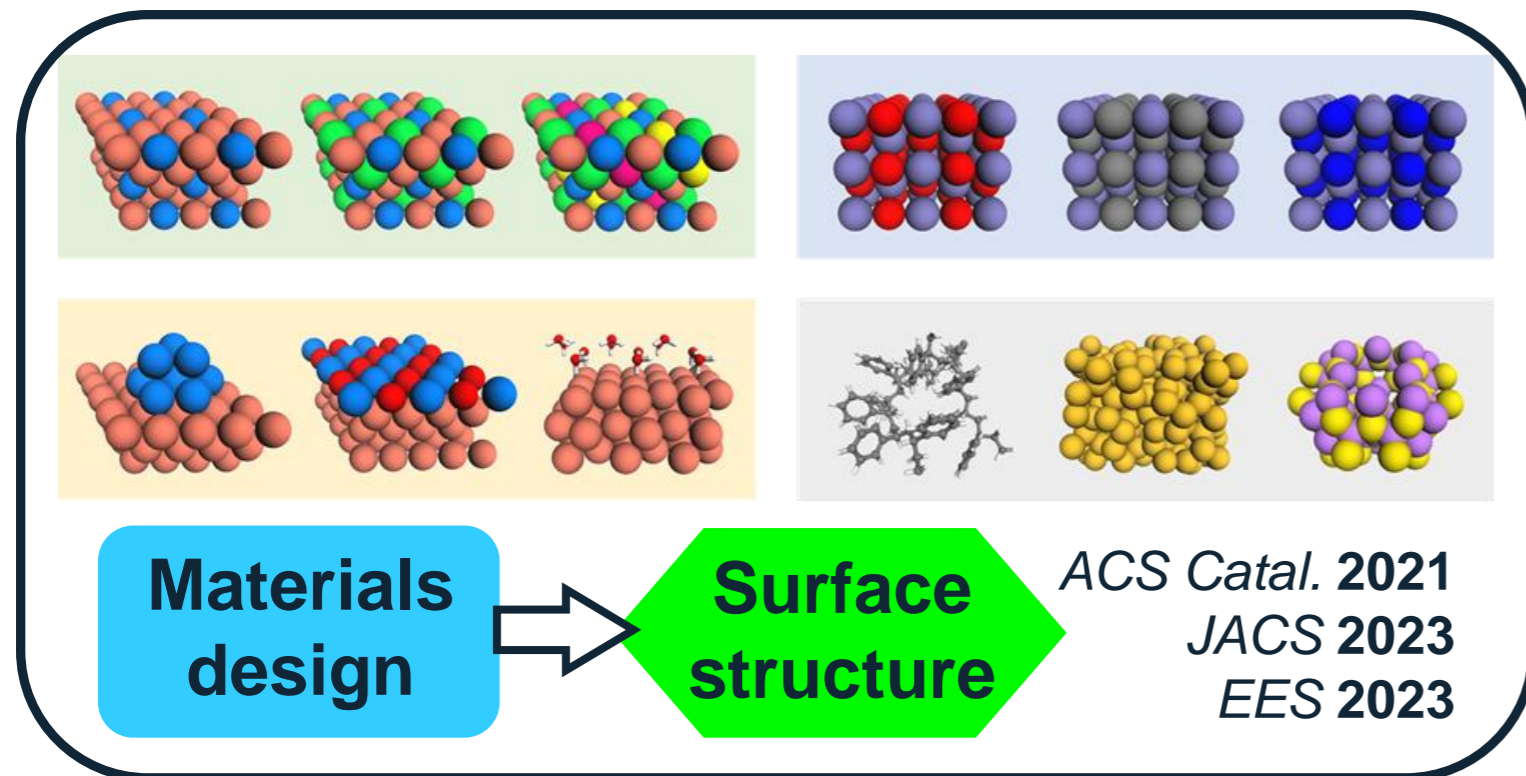
Customer Support

Literature processing

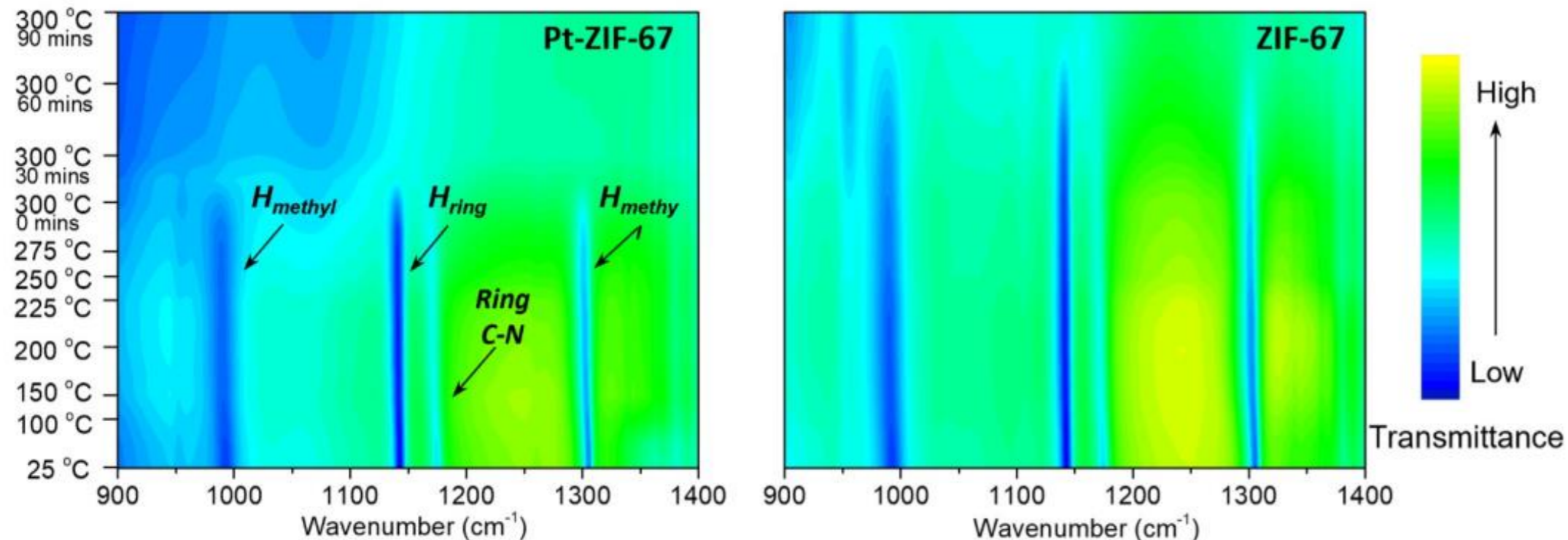
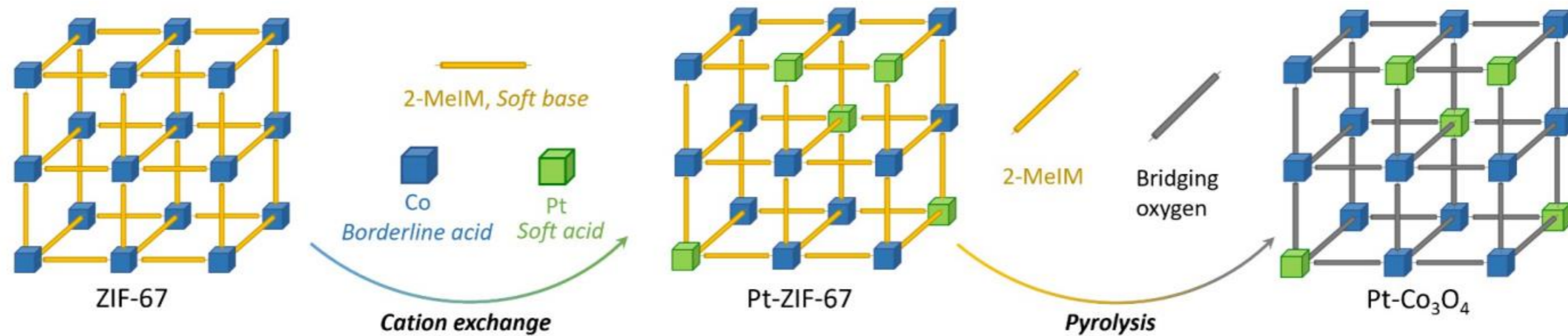
Database and ideas



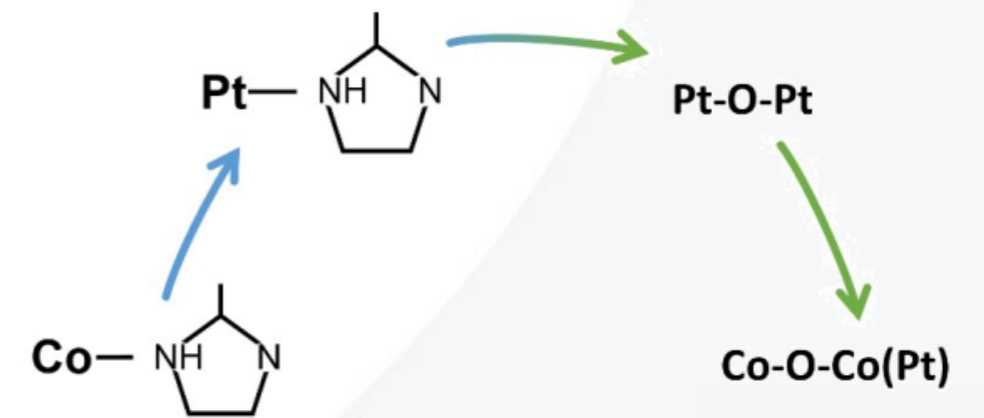
# AI applications: What can we do now?



# Single-atom catalyst formation mechanism

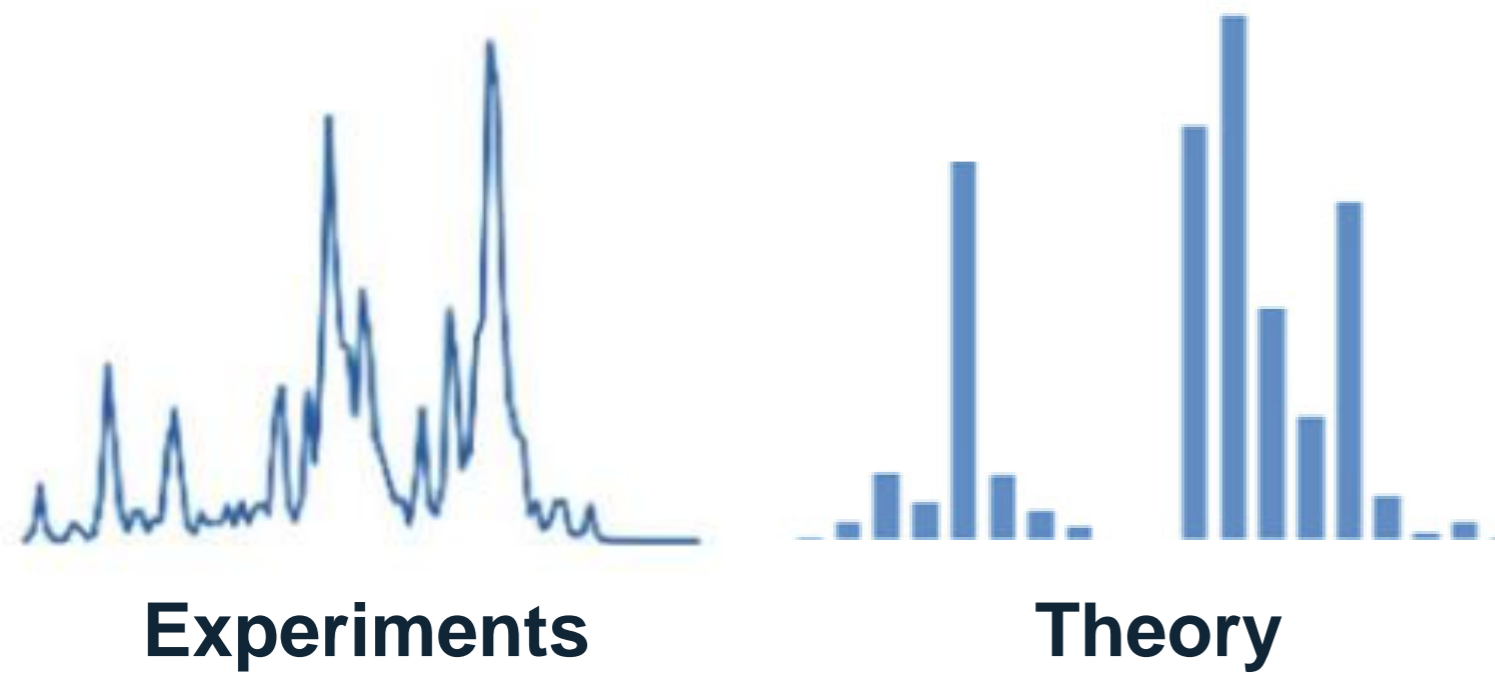


## Experimental mechanism: Infrared spectroscopy

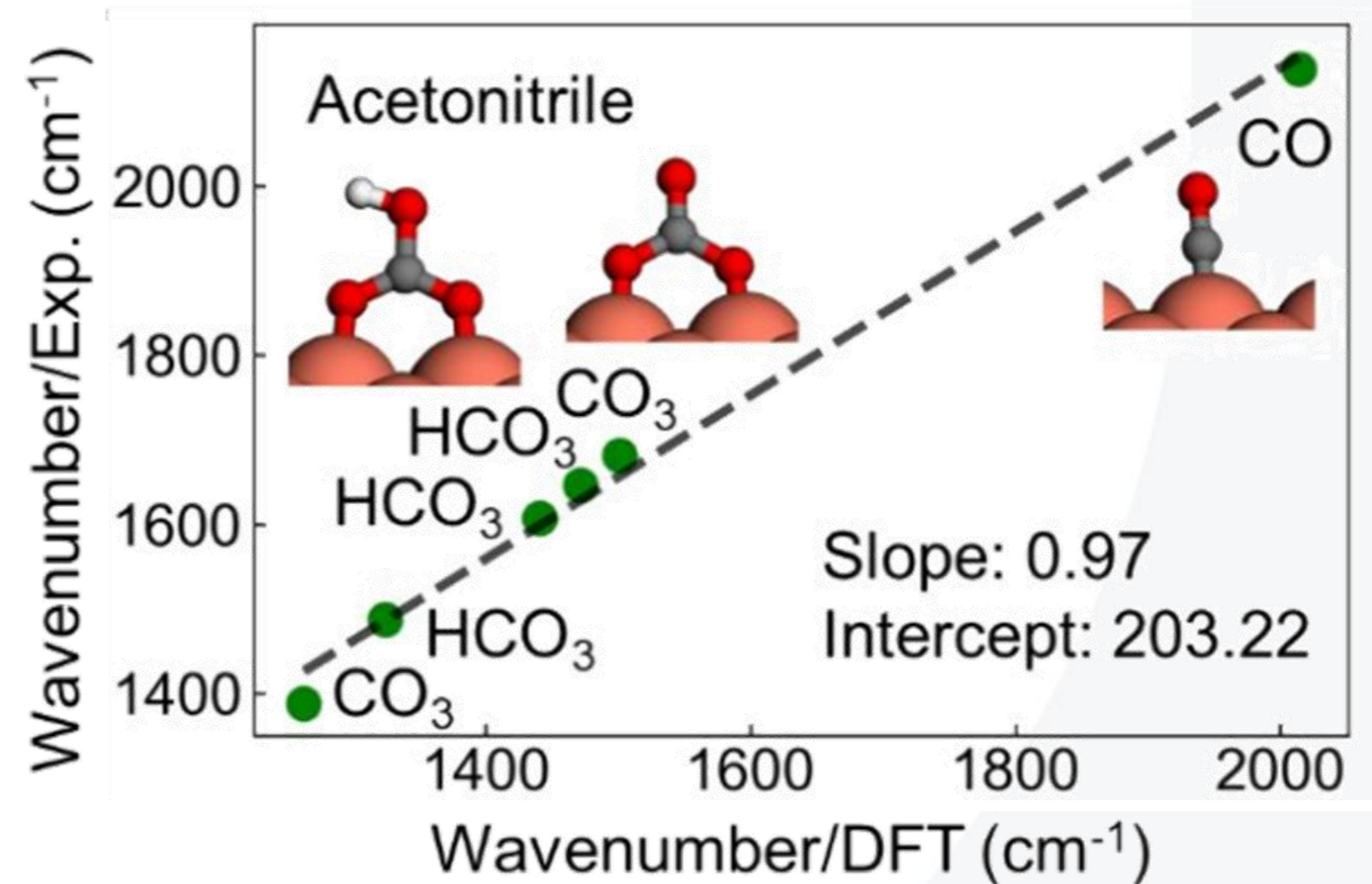


# Infrared spectroscopy simulation

Challenge:  
*Gap between experiments and theory*

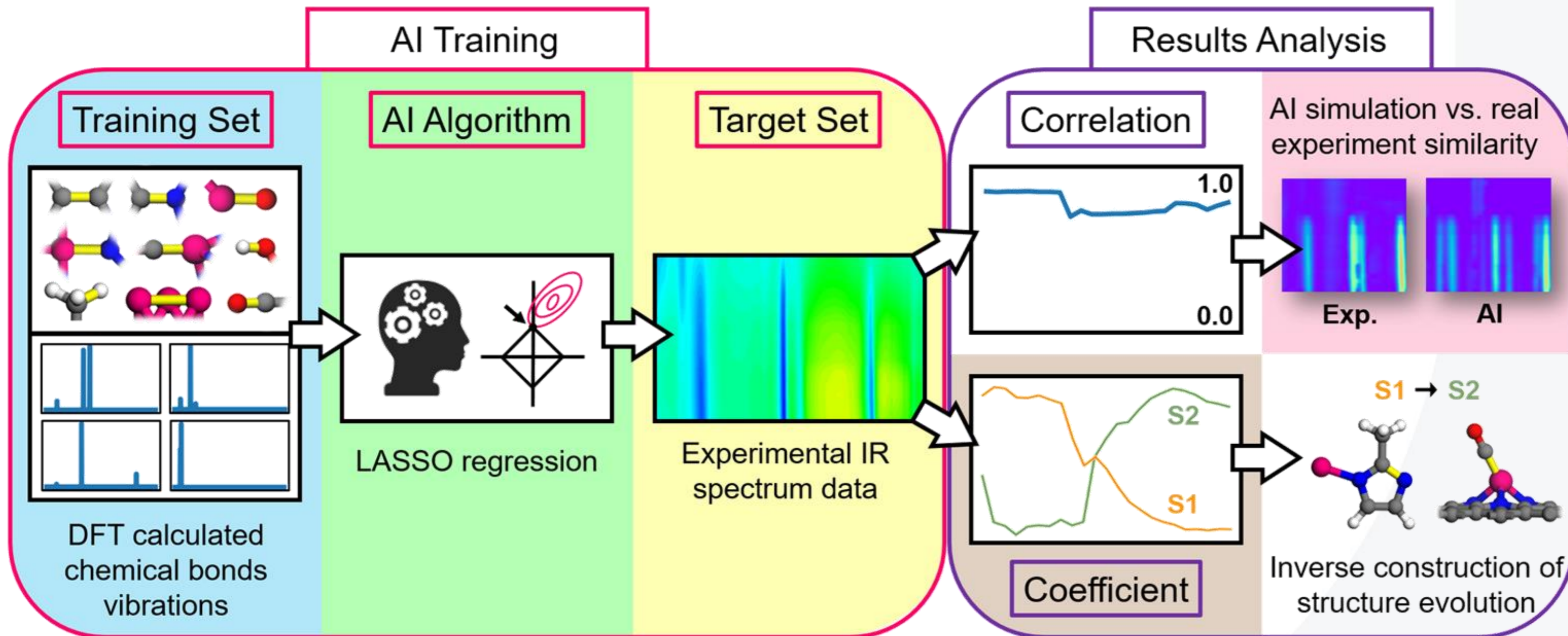


*Linear relationship between calculated and experimental wavenumbers*



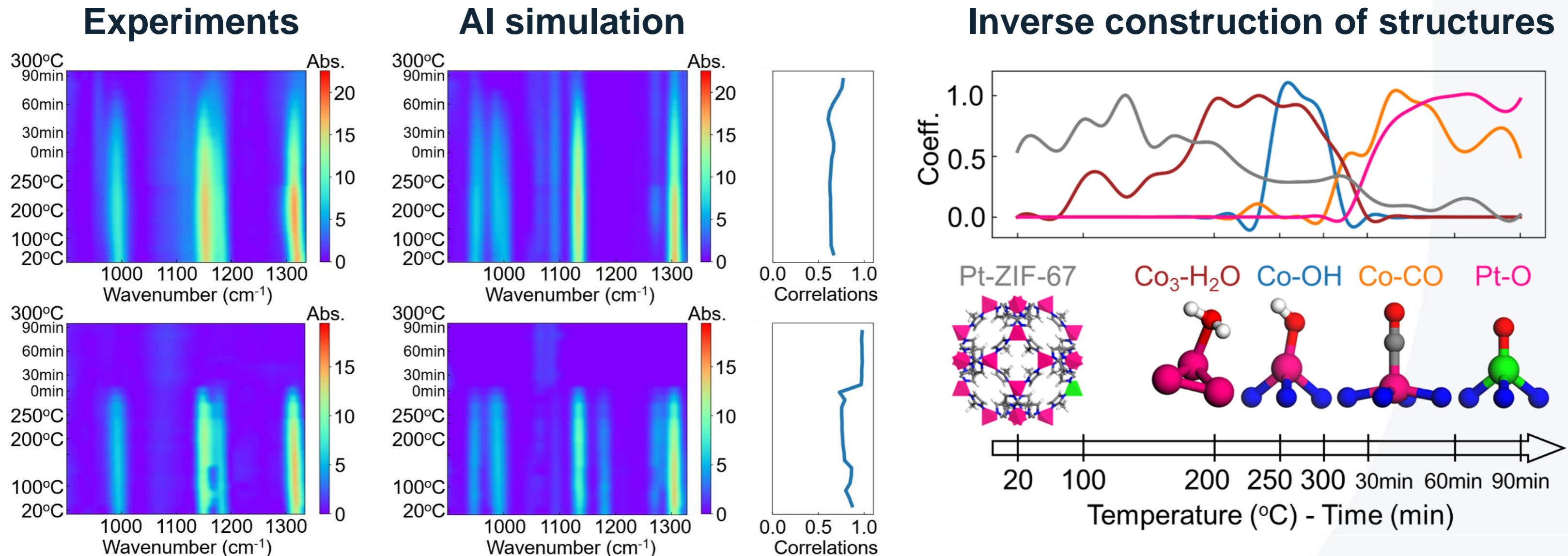
*Use AI algorithm (linear regression) to bridge this gap!*

# Workflow development



*First use AI technique to analyze in-situ experimental spectroscopy*

# AI-driven reaction mechanism analysis



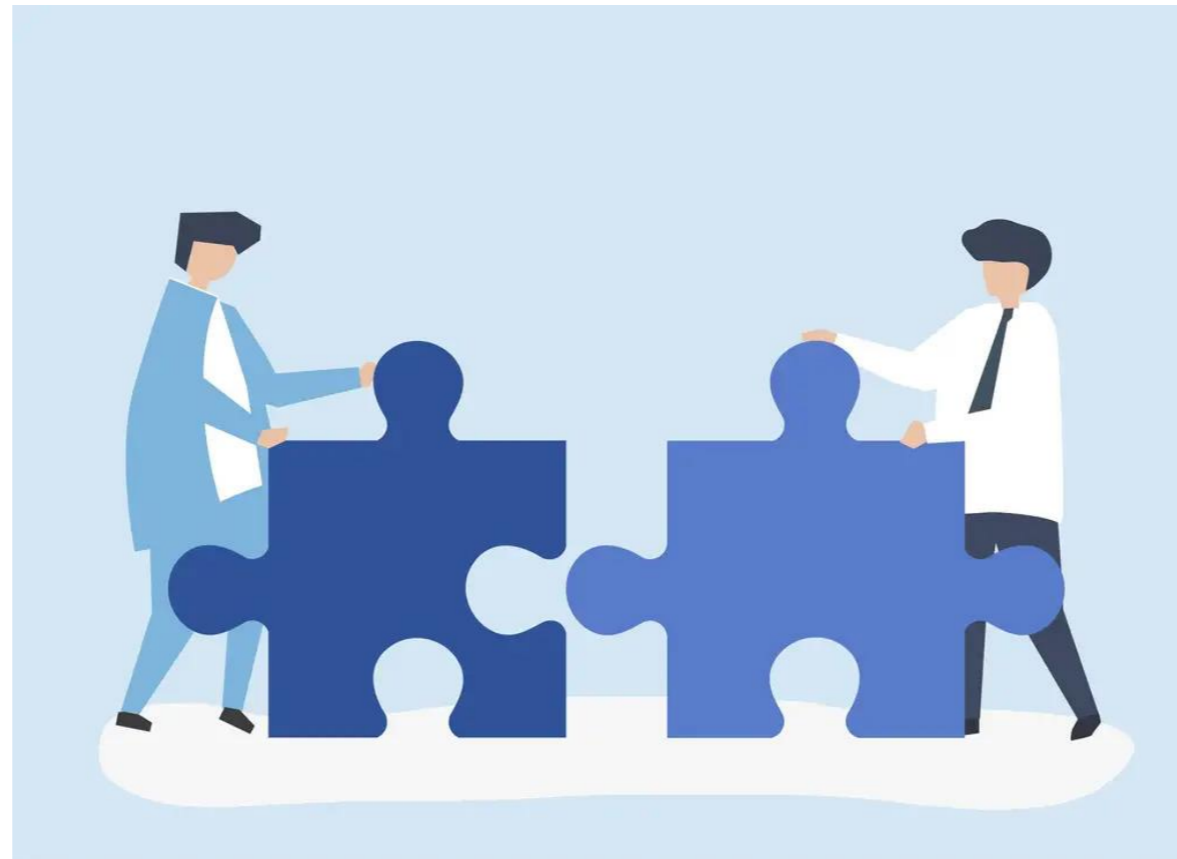
*AI can effectively simulate real experimental data, and deduce chemical reaction mechanisms for the pyrolysis process that align with manual experimental analysis.*



# Outlook

*In-situ* spectroscopy data: IR, Raman, XRD, XAS, ...

Working conditions: Temperature, electrochemical potential, pH, solvents...



# Thanks for the attention!

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**Alexander von Humboldt**  
Stiftung/Foundation



**Australian Government**  
**Australian Research Council**



**THE UNIVERSITY**  
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**Haobo Li**

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*We're not just researchers, we are community of brilliant minds.*

