Accelerating Scientific Discovery in Catalysis with Artificial Intelligence

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AIMS Workshop, NIST

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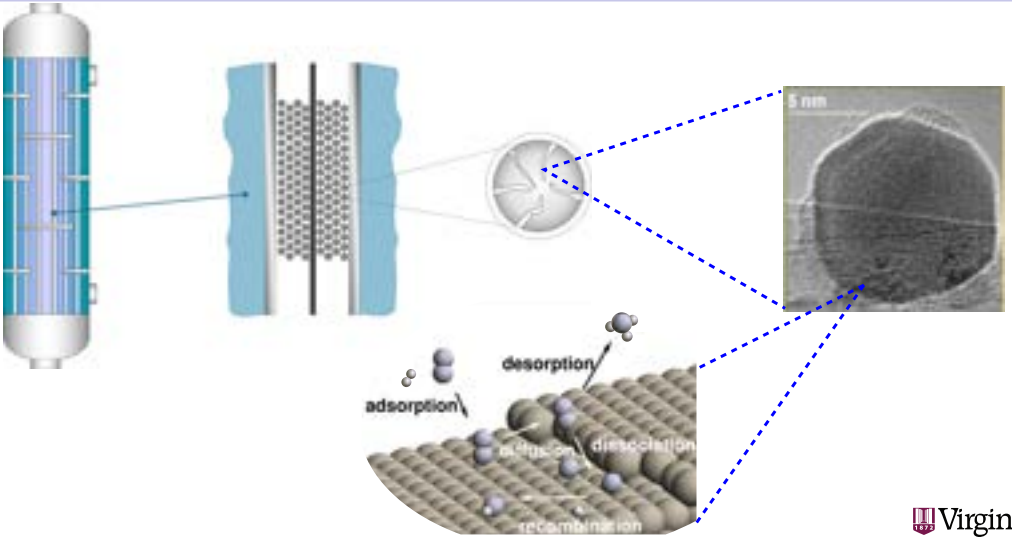
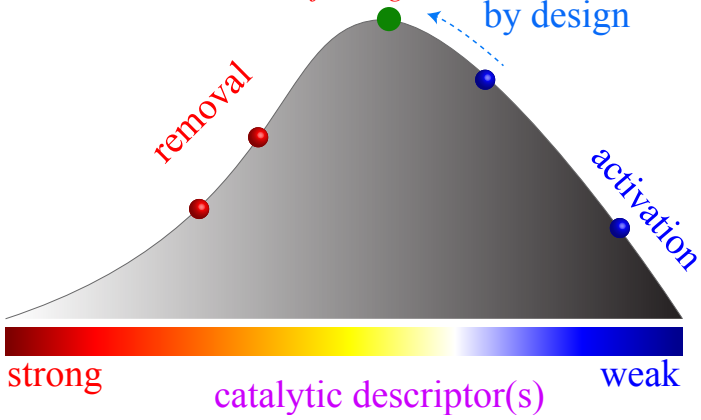
VirginiaTech

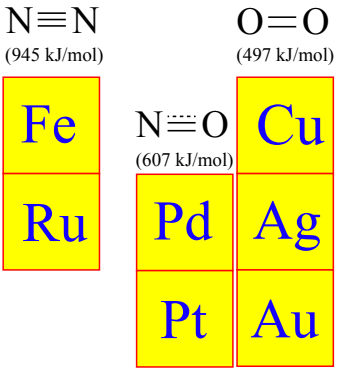
A multiscale perspective in heterogeneous catalysis



Chemistry and material challenges

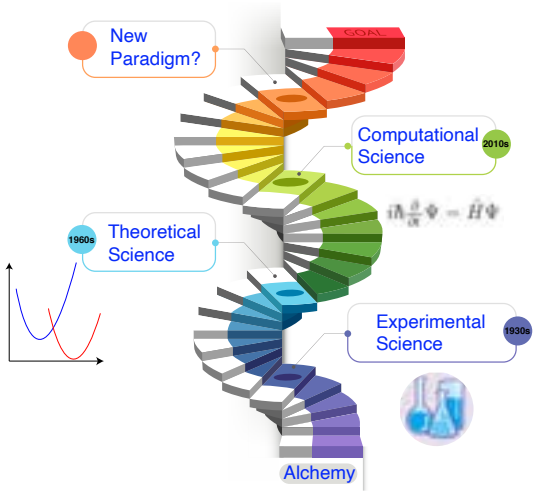
The Sabatier principle states that the interactions between the catalyst and key intermediates should be just right; that is, neither too strong nor too weak.





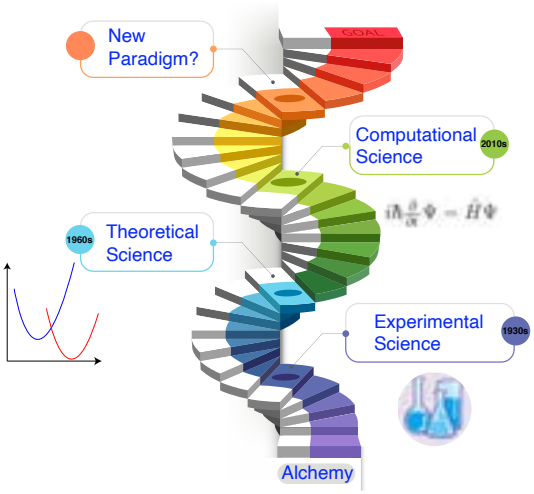
Nørskov, et al., Fundamental Concepts in Heterogeneous Catalysis, 2014.

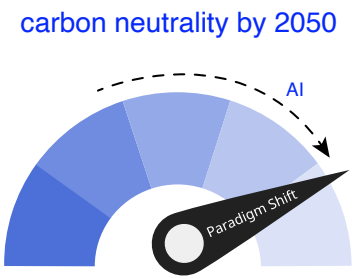
Evolving paradigms of catalytic materials discovery



H. Xin, T. Mou, H. S. Pillai, S.-H. Wang, Y. Huang, Acc. Mater. Res. 5, 22-34 (2024).

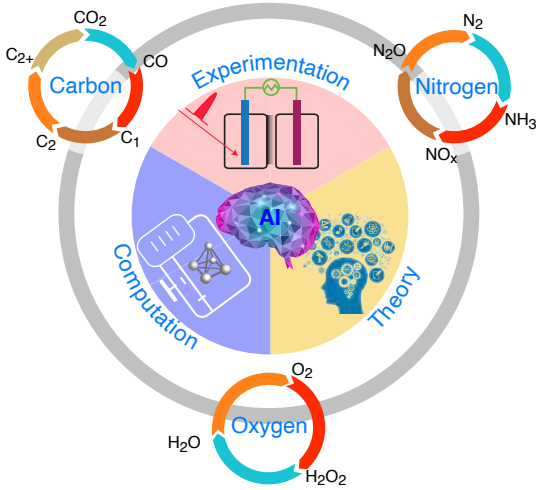
Evolving paradigms of catalytic materials discovery

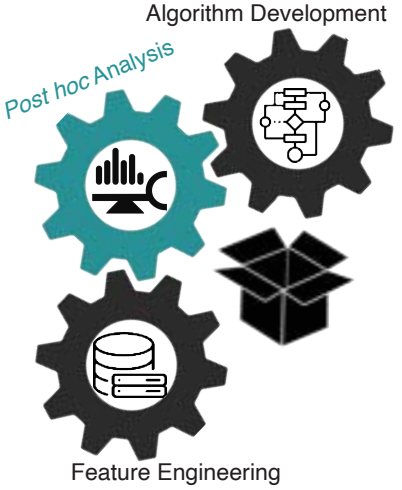




H. Xin, T. Mou, H. S. Pillai, S.-H. Wang, Y. Huang, Acc. Mater. Res. 5, 22-34 (2024).

Catalyzing the transition to a circular economy with AI





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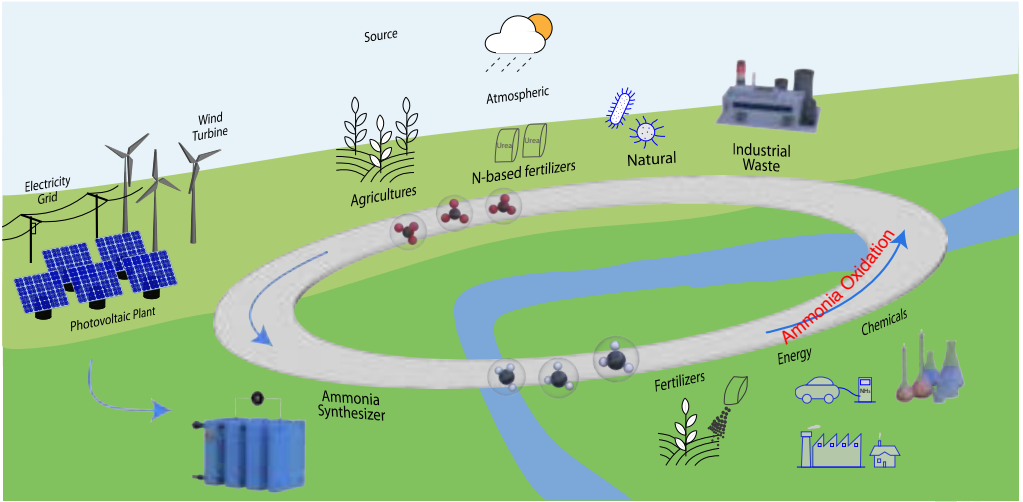
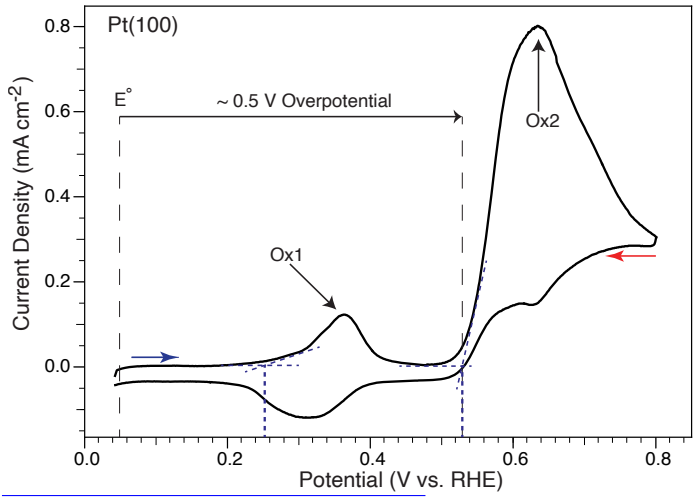
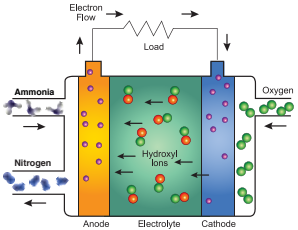
Toward a sustainable nitrogen cycle through catalysis



Cyclic voltammetry of NH_3 oxidation on Pt(100)





$$2NH_3 + 6OH^- \rightarrow N_2 + 6H_2O + 6e^-$$

Exp. onset potential: +0.53 V_{RHE}

$$NH_3 + 2{*}H + 2OH^- \rightarrow {*}NH_3 + 2H_2O + 2e^-$$

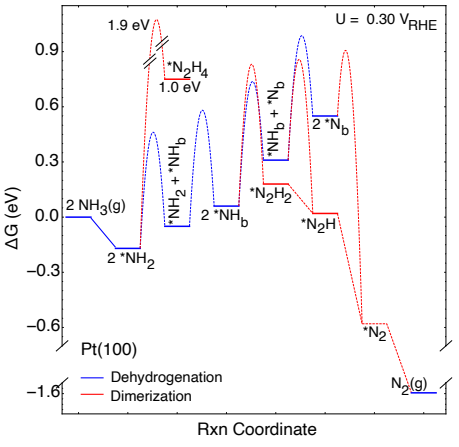
Exp. onset potential: +0.25 V_{RHE}

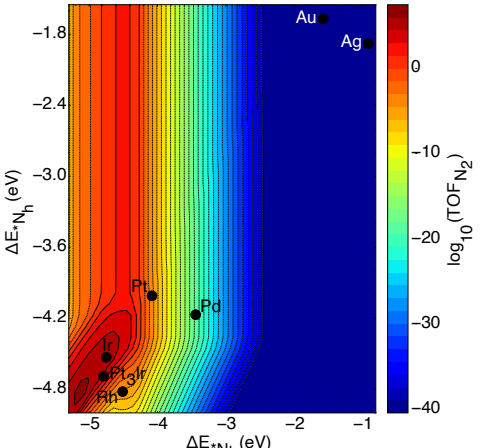
Surface deactivation: ~+0.6 V_{RHE}

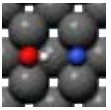
Katsounaros, et al., J. Catal., 359, 82-91, (2018).

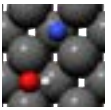
Mechanistic understanding of AOR at metal surfaces

$$2NH_3 + 6OH^- \rightarrow N_2(g) + 6H_2O + 6e^- \quad (E^0 = +0.05\ V_{RHE})$$





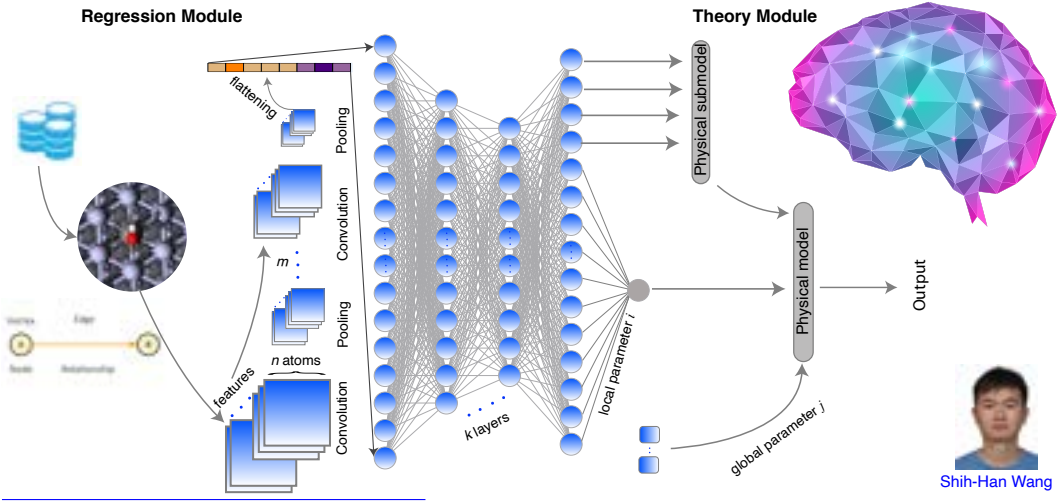

*N_b


*N_h


Hemanth Pillai

H. S. Pillai, Y. Li, S. Wang, N. Omidvar, et al., Nat. Commun. 14, 1 (2023).

Developing a theory-infused neural network (TinNet)



Shih-Han Wang

https://github.com/hlxin/tinnet

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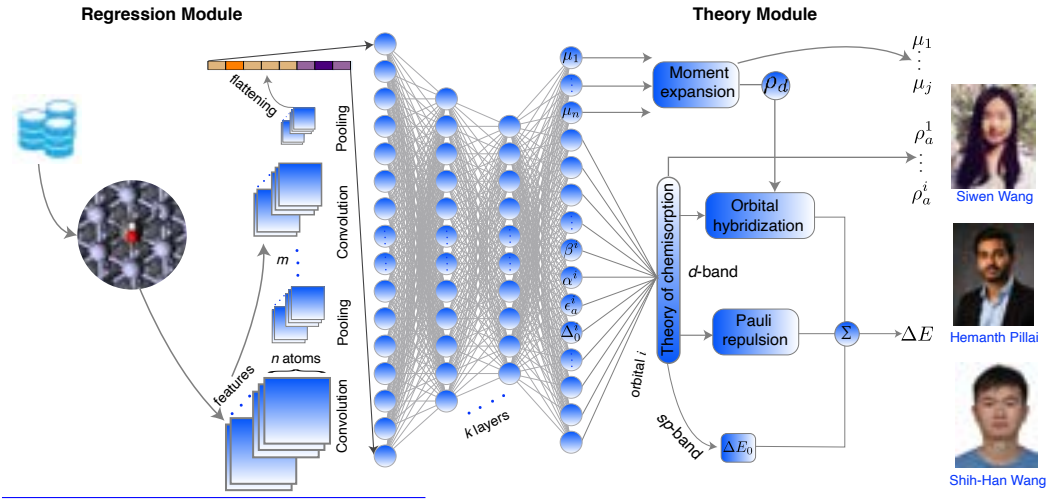
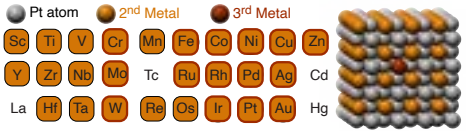
A TinNet framework integrated with the *d*-band theory



B. Hammer, J. Nørskov, Surf. Sci. 343, 211 (1995); Shih-Han Wang, et al., Nat. Commun. 12, 5288 (2021).

Rapid screening of Ir-free, ternary Pt alloys for AOR

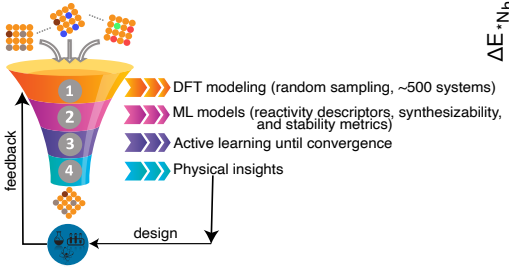


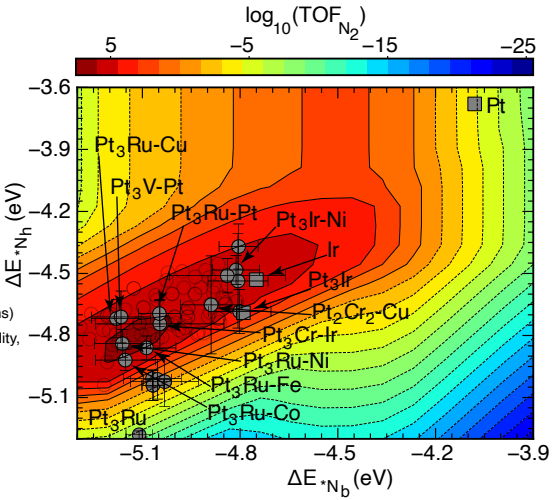
2 bulk Pt_3M and PtM with 25 M metals

3 Surface terminations for the {100} facet

15 3rd metal in 8 possible positions ~24k adsorbate configurations

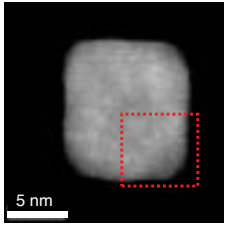
2 Adsorbates with up to 2 adsorption sites

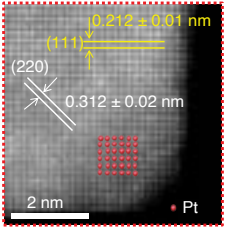


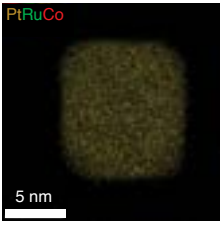


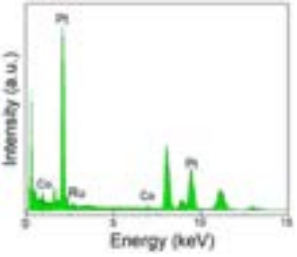
H. S. Pillai, Y. Li, S. Wang, N. Omidvar, et al., Nat. Commun. 14, 1 (2023).

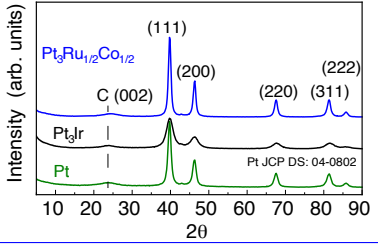
Successful synthesis of $Pt_3Ru_{1/2}Co_{1/2}$ alloy nanocubes

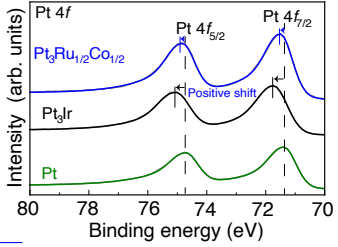












Gang Wu

Yi Li

H. S. Pillai, Y. Li, S. Wang, N. Omidvar, et al., Nat. Commun. 14, 1 (2023).

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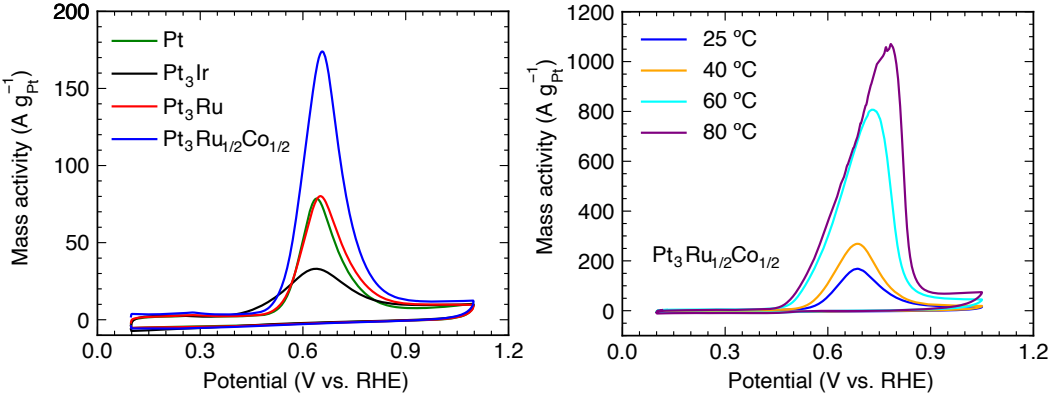
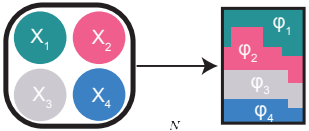
Experimental validation of model-predicted ternary alloys



- $Pt_3Ru_{1/2}Co_{1/2}$ has the highest peak current density of 174.0 mA mg^{-1} Pt, higher than pure Pt (78.6 mA mg^{-1} Pt) and Pt_3Ir.

H. S. Pillai, Y. Li, S. Wang, N. Omidvar, et al., Nat. Commun. 14, 1 (2023).

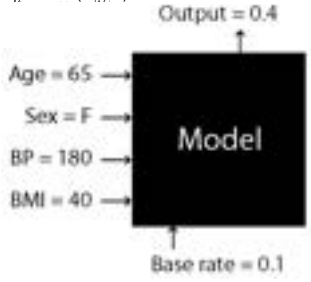
Opening the black box of machine learning models

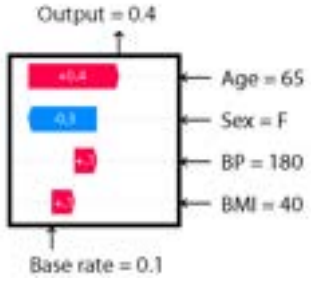


$$g(x') - \varphi_0 - \sum_{i=1}^{N} \varphi_i x_i'$$

$$\varphi_i(v) = \frac{1}{n} \sum \binom{n-1}{|S|}^{-1} (v(S \cup \{i\}) - v(S))$$

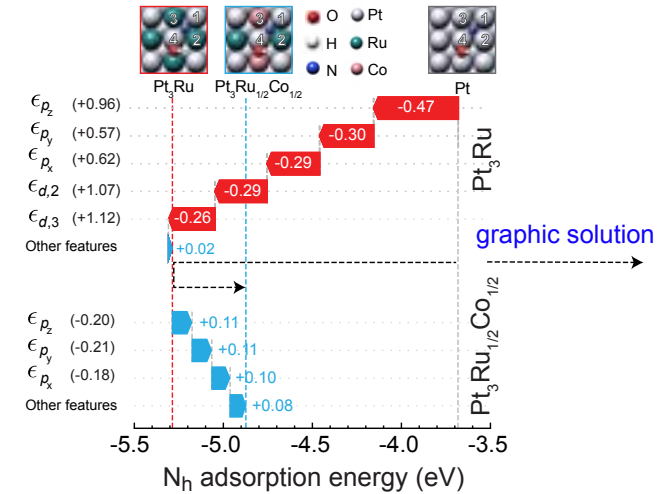
SHAP (SHapley Additive exPlanations) explains the prediction of an instance by computing the contribution of each feature (Shapley value) to the prediction, rooted in cooperative game theory.



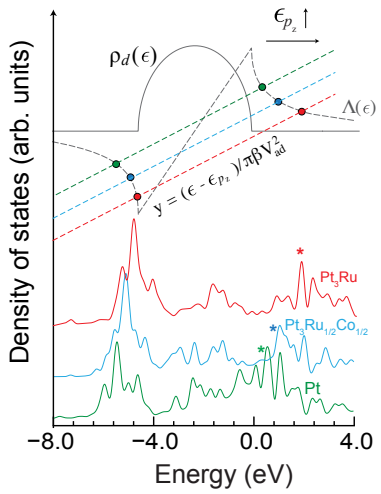


Lundberg, S. M.; Lee, S.-I. Adv. Neural Inf. Process. Syst. 2017, 30, 4765-4774.

SHAP analysis for deep insights into chemical bonding

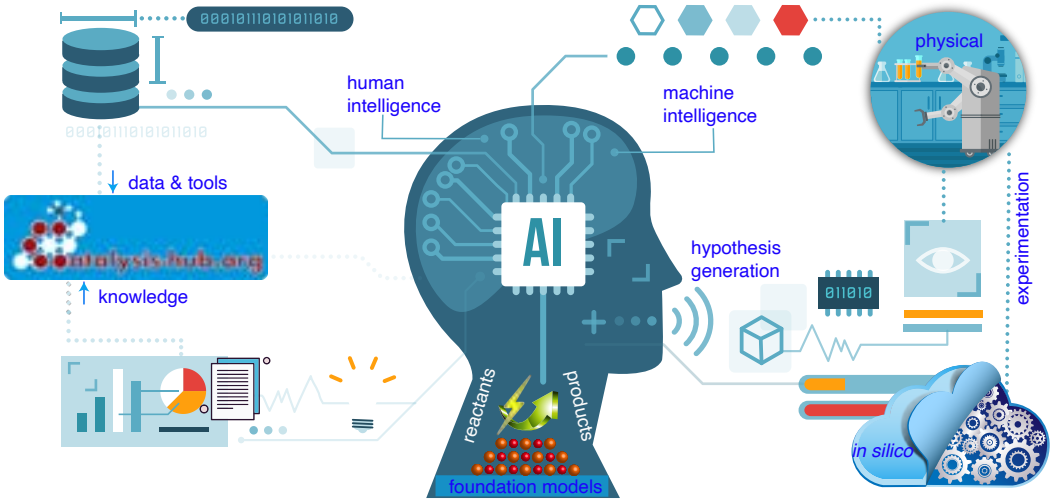


graphic solution



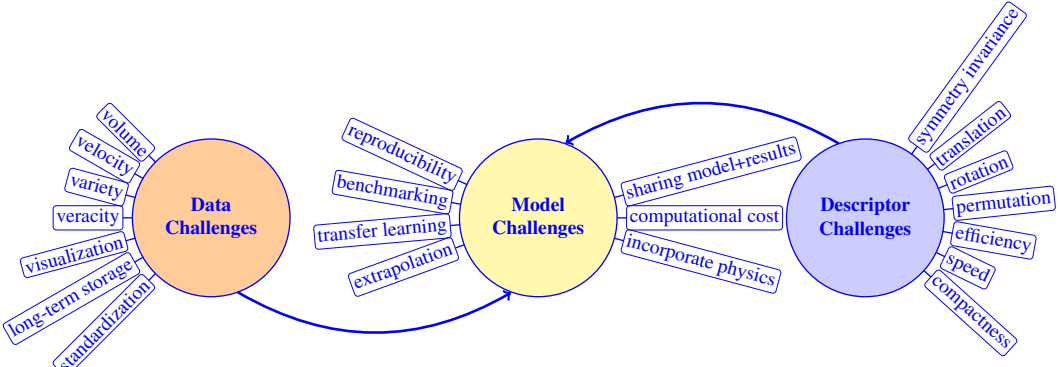
H. S. Pillai, Y. Li, S. Wang, N. Omidvar, et al., Nat. Commun. 14, 1 (2023).

AI scientists in catalysis, a possibility or fantasy?



AIMED Workshop on Heterogeneous Catalysis, Oct. 10-11, 2024. (https://aimedx.github.io/hetcat).

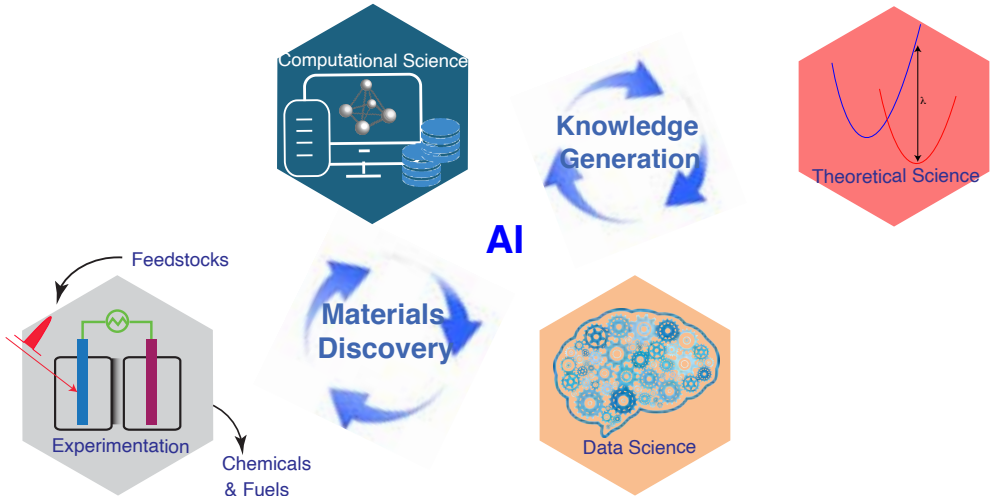
Challenges in developing AI scientists



1. Data: Data ecosystems that follows the FAIR principle.
2. Descriptors: Hierarchical representations of systems.
3. Models: Hybridizing deep learning with domain knowledge.

Mou, T.; Pillai, H. S.; Wang, S.; et al., Nat. Catal. 2023, 6 (2), 122-136.

Conclusions



Acknowledgement

Collaborators


Huiyuan Zhu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Rong Tong


Xingchen Ye


Fudong Liu


Fanglin Che

And all my current and former students!