

2025年05月09日

人工智能算法与原理

智能驱动物理规律提取和数学公式构建算法

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中国科学技术大学
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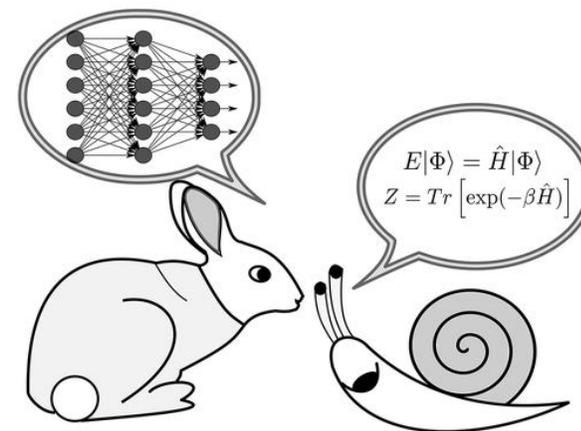
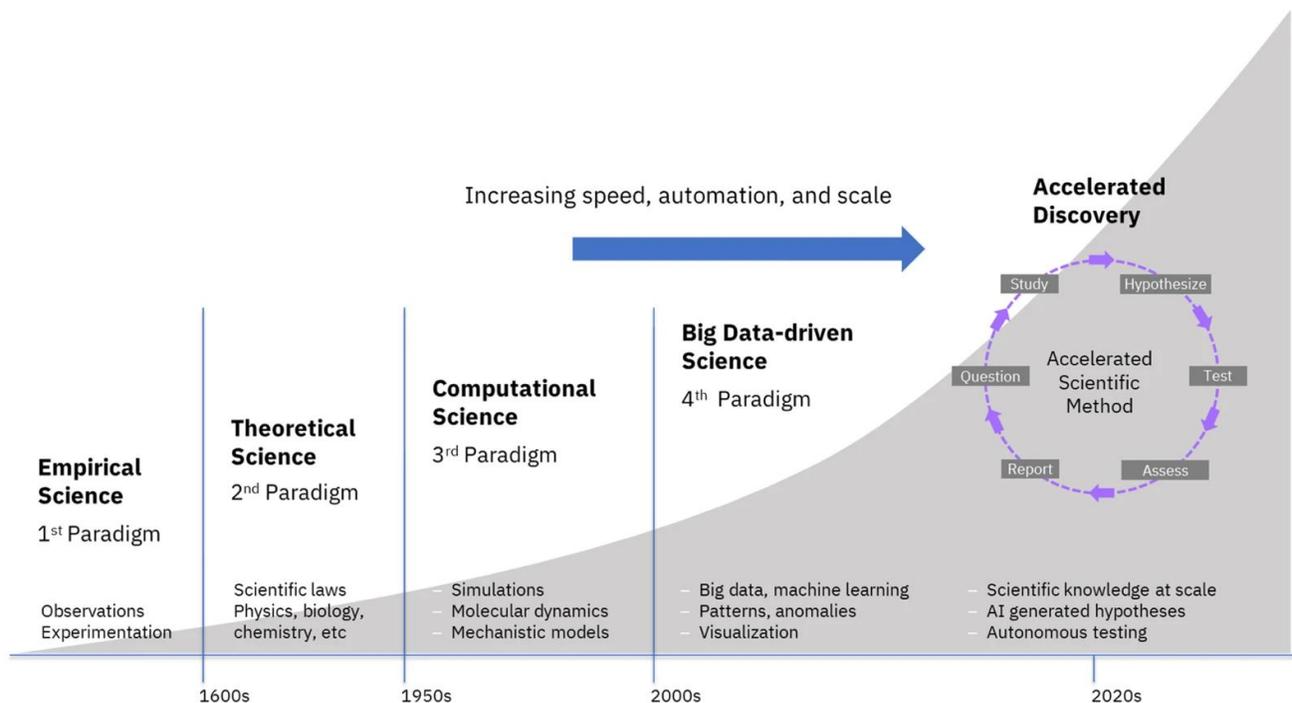
合肥微尺度物质科学国家研究中心
HEFEI NATIONAL LABORATORY FOR PHYSICAL SCIENCES AT THE MICROSACLE

科学范式迁移变革催化研究进程

- 相关性与因果性
- 物理规律的提取

- 规则与材料基因
- 数据挖掘与预测

- 统计与概率分布
- 高维势能面鞍点和极小



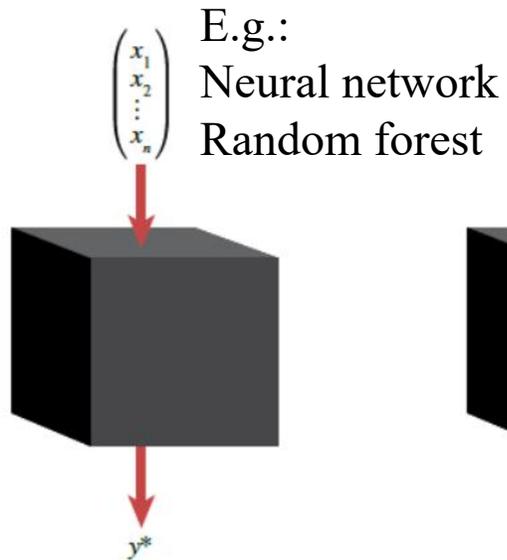
DFT精度机器学习势函数模拟大体系

E. O. Pyzer-Knapp, A. Curioni, Npj Comput Mater 8(2022) 84

Parrinello, Phys Rev Lett 98 (2007) 146401

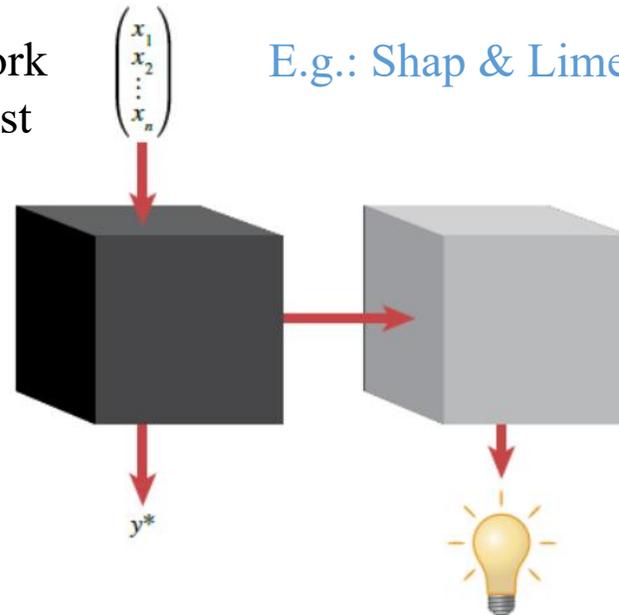
Interpretable Machine Learning

“Black box”



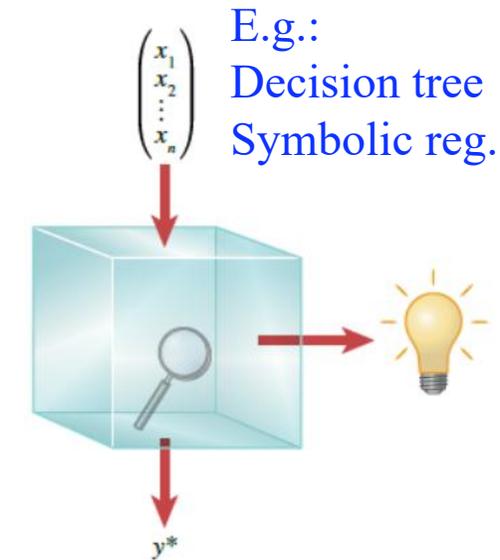
Prediction

“Grey box”



**Prediction &
Post hoc explanation**

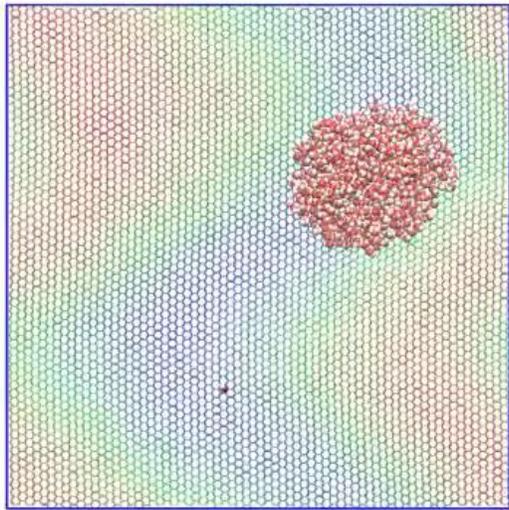
“Glass box”



**Prediction &
Intrinsic interpretability**

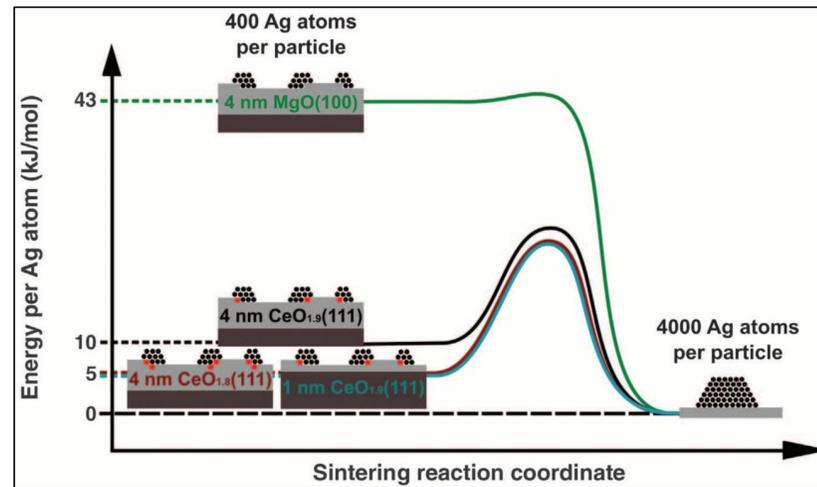
原子到宏观尺度材料结构演化动力学过程

催化剂扩散团聚失活



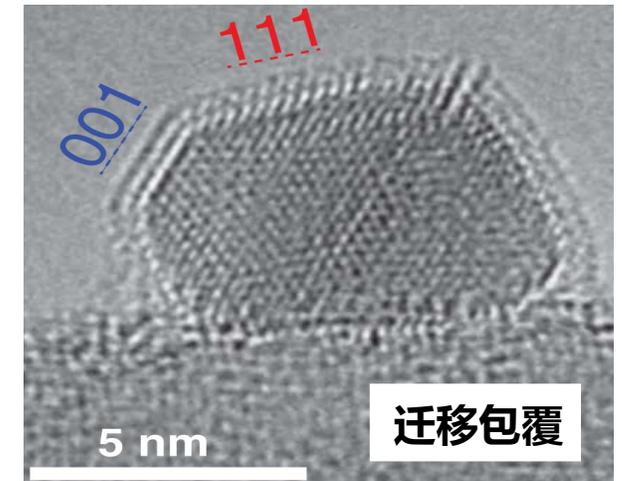
Nat. Mater. 2016, 15, 66.

催化剂Ostwald熟化失活



Science, 2010, 329, 933.

氧化物迁移包覆



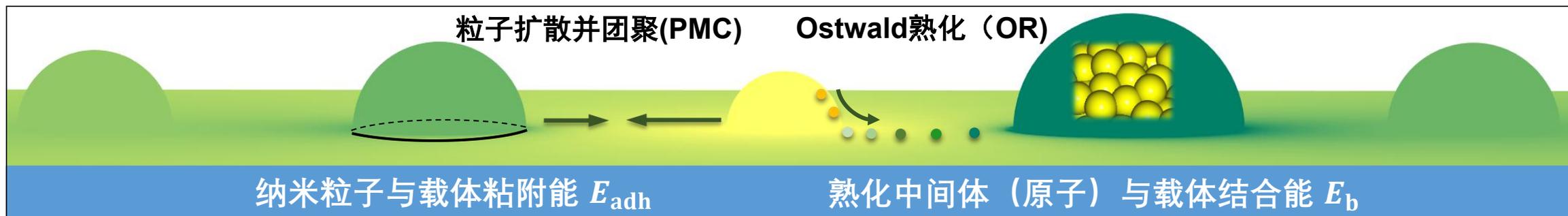
Science, 2022, 376, 982.

其他失活机制：相变、偏析、分散、溶解、中毒、积碳

重要性：对于实验室纳米催化剂工业应用和产业化生死攸关

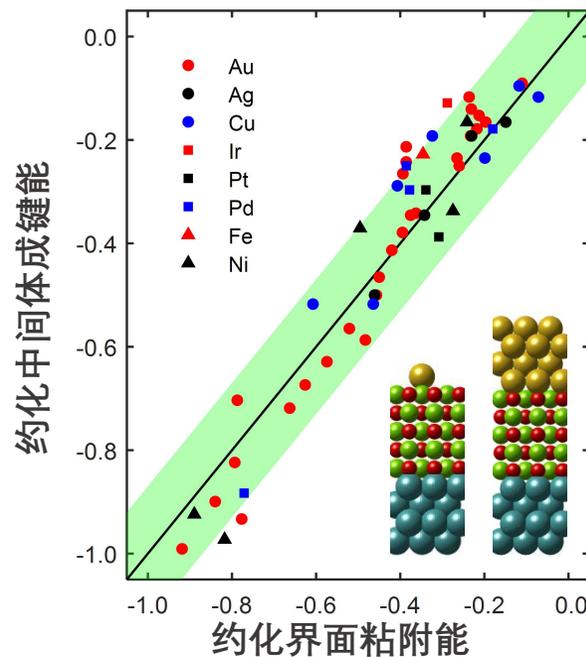
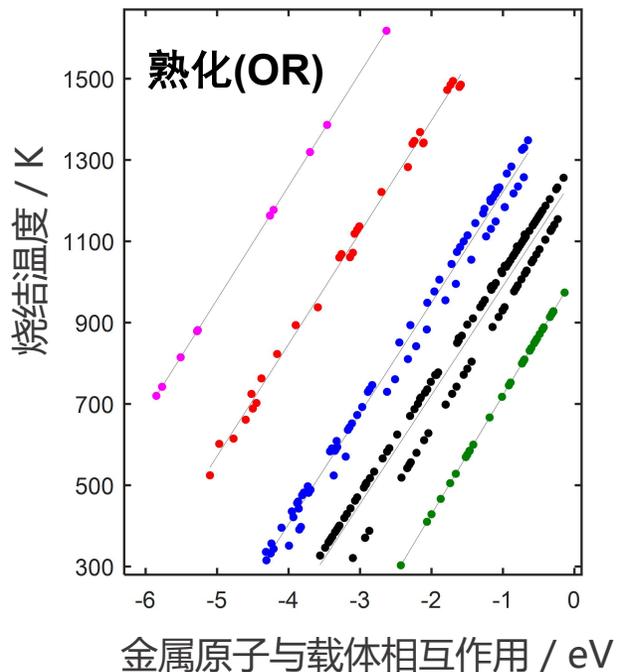
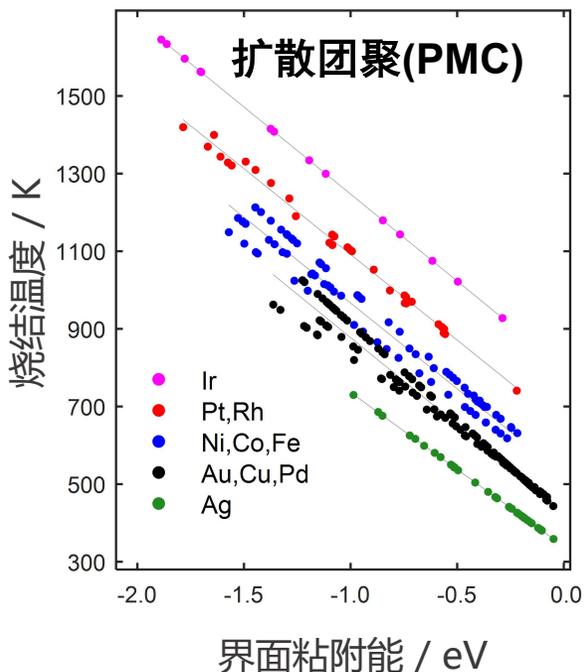
核心目标：揭示催化剂失活动力学标度关系/竞争规律/协同原理，建立理论公式模型

烧结动力学标度关系和界面粘附-原子成键标度关系



$$\frac{\partial f(v,t)}{\partial t} = \int_0^v D(v') f(v',t) f(v-v',t) dv' - \int_0^v [D(v) + D(v')] f(v,t) f(v',t) dv'$$

$$\frac{dr}{dt} = \frac{AB}{A+B} \frac{v_p \Omega}{4\pi a^2 \alpha_1 r^2} \exp\left(-\frac{E_{tot}}{kT}\right) \left[\exp\left(\frac{2\gamma_m \Omega}{kTr^*}\right) - \exp\left(\frac{2\gamma_m \Omega}{kTr}\right) \right]$$

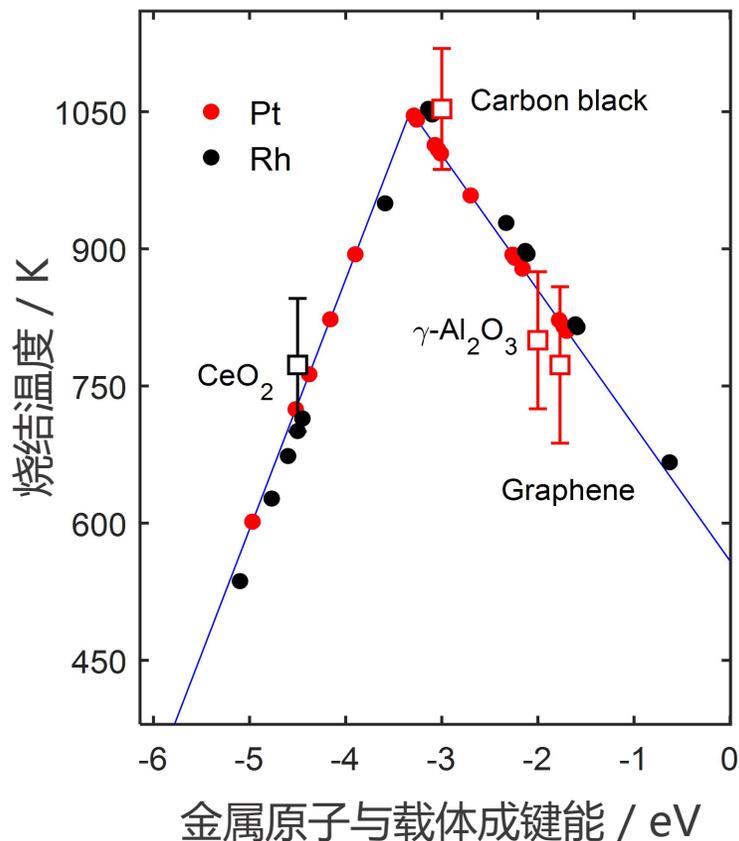
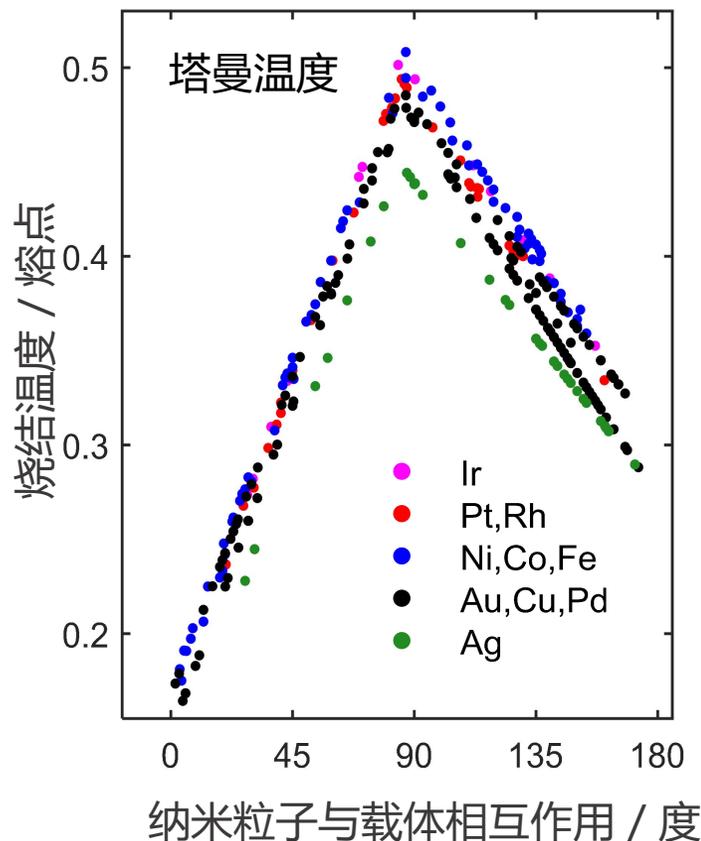


$$\frac{E_{adh}}{2\gamma_m} = - \frac{E_b}{E_c}$$

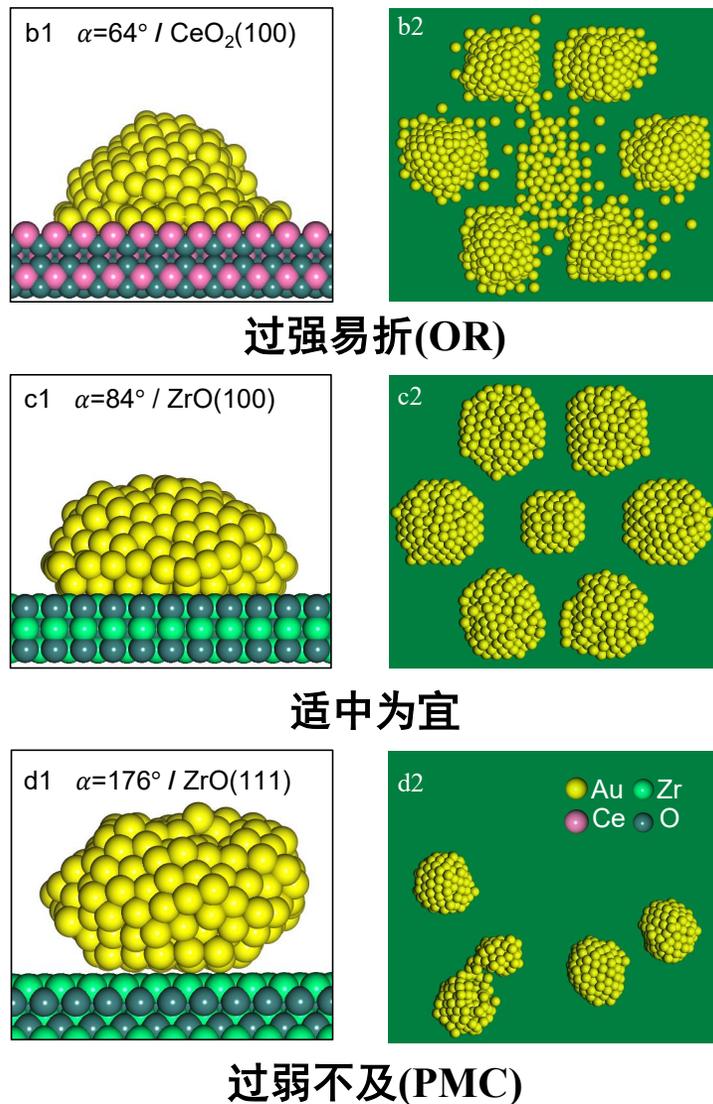
粘附能 / 表面能 = 成键能 / 内聚能

界面粘附决定的抗烧结稳定性Sabatier普适竞争原理

数据驱动 (1252个能量学, 302种金属-载体组合)

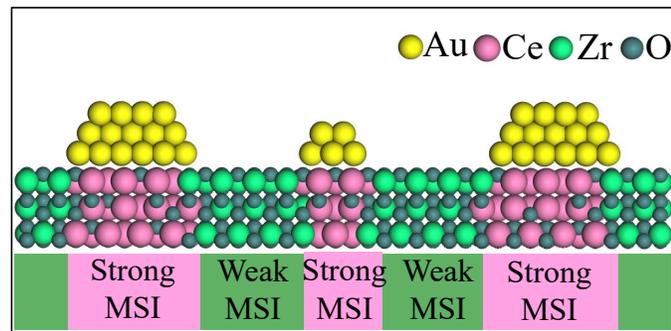


第一性原理神经网络势分子动力学模拟

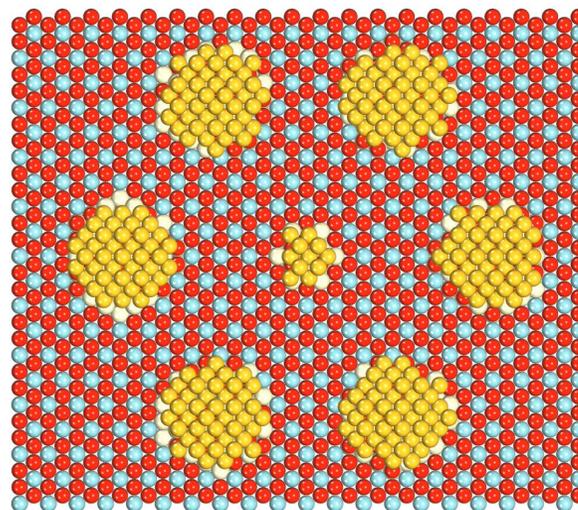


纳米催化剂抗烧结热稳定性普适性火山型关系及验证

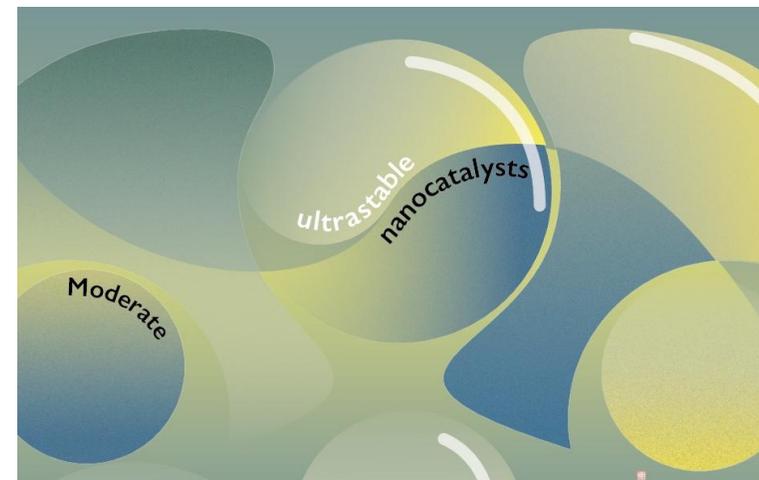
打破界面标度超越Sabatier原理-双功能载体协同设计



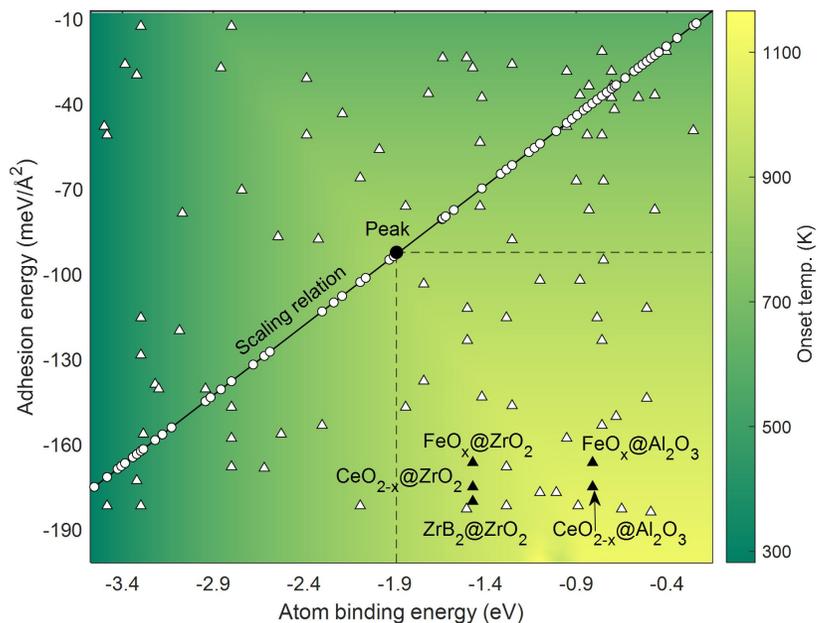
双功能载体设计



神经网络势分子动力学
800 K, LASP



适中为宜 (单组份) vs. 强弱融合(双功能)



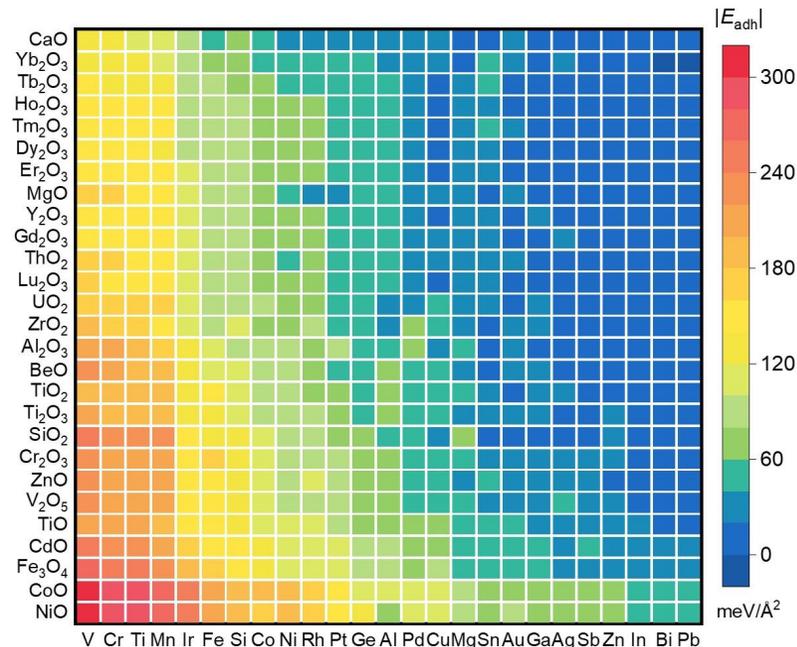
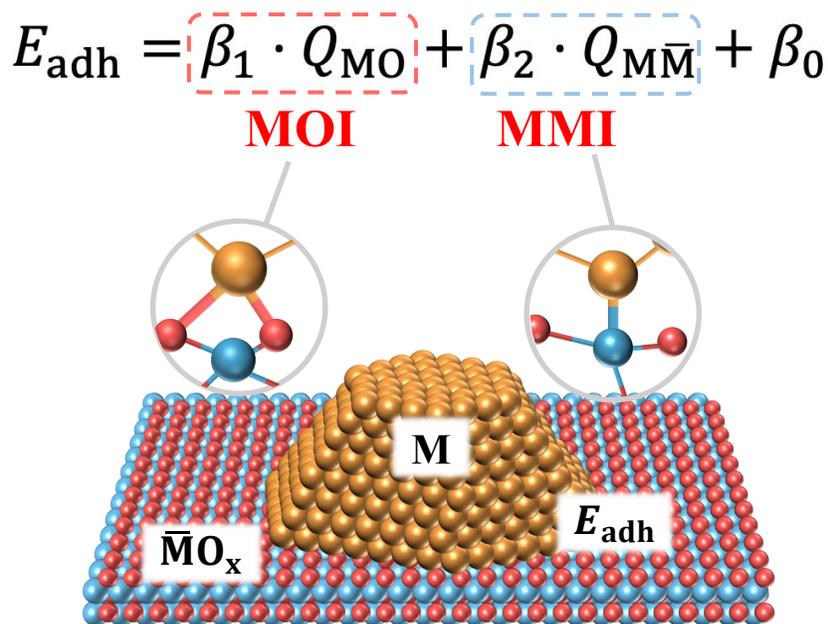
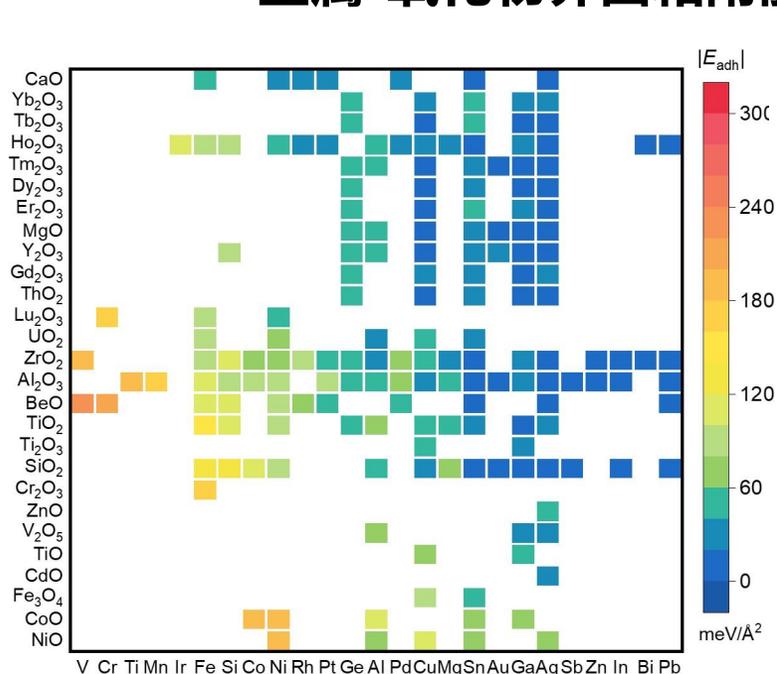
高通量筛选 (6724种)

- 耐受温度远超塔曼温度，甚至接近熔点温度
- 为理论设计超稳定催化剂奠定了重要科学基础

Hu, Li*, *Science*, 2021, 374, 1360-1365.

金属-氧化物界面相互作用本质及预测公式

金属-氧化物界面粘附能



压缩感知SISSO机器学习方法

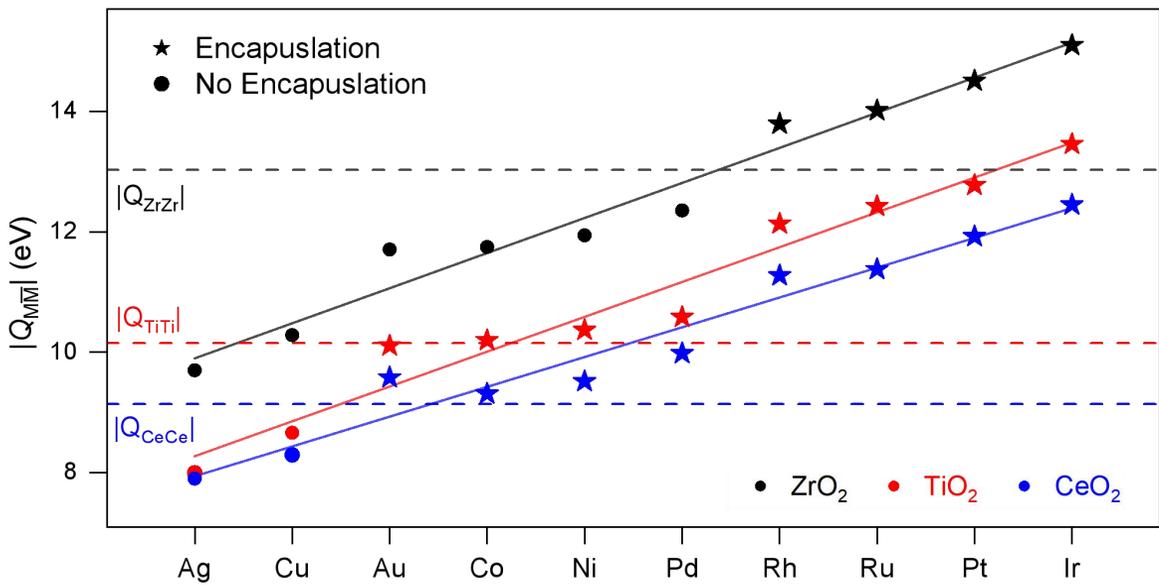
金属-氧键 $Q_{MO} = \Delta H_f^{MO} - \Delta H_{sub}^M$,

金属-金属键 $Q_{MM} = \Delta H_f^{MM} - \Delta H_{sub}^M - \Delta H_{sub}^M$

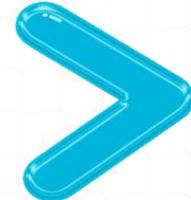
金属-氧化物界面作用由金属与氧的亲合性以及金属-金属亲合性共同决定

Wang[#], Hu[#], Ouyang[#], Hu, Li*, Science 2024, 386, 915.

金属-金属键竞争决定的氧化物包覆催化剂的理论判据



负载金属与氧化物金属键 $|Q_{MM}|$



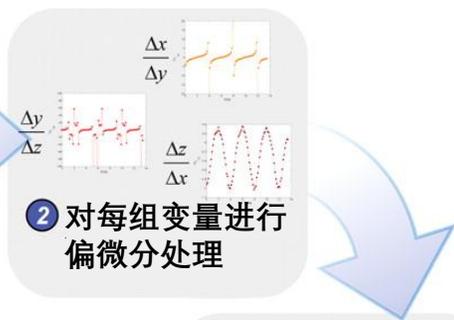
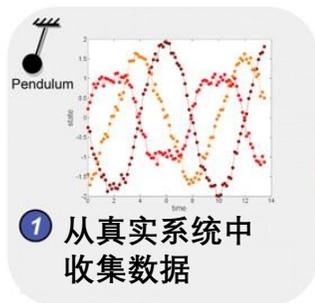
氧化物金属与氧化物金属键 $|Q_{MM}|$

金属-金属键 $Q_{MM} = \Delta H_f^{MM} - \Delta H_{sub}^M - \Delta H_{sub}^{\bar{M}}$

- 10 Late TMs
- 16 Oxides: Nb₂O₅, Ta₂O₅, Fe₃O₄, TiO₂, CeO₂, ZnO, ZrO₂, Al₂O₃, SiO₂, MgO...

Wang#, Hu#, Ouyang#, Hu, Li*, Science 2024, 386, 915.

符号回归对于科学模型构建的探索



3 产生候选方程, 方程参数随机

$$f = (x - 1.12) \cdot \cos(y)$$

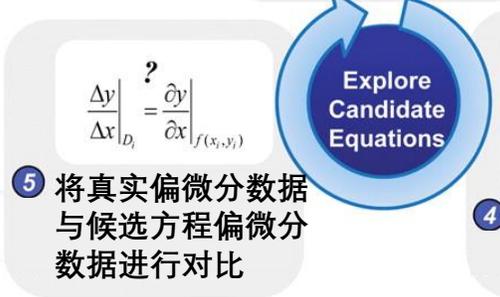
$$f = 0.91 \cdot \exp(y/z)$$

$$f = 0.5 \cdot y^2 - 9.8 \cdot \cos(x)$$

6 得到误差范围内允许的方程

$$f = z + 9.8 \cdot \sin(x)$$

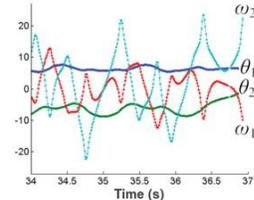
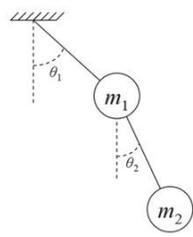
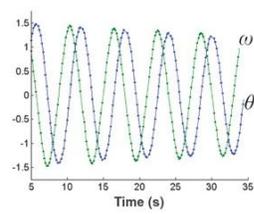
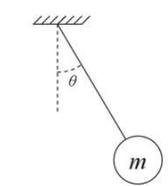
$$f = 0.5 \cdot y^2 - 9.8 \cdot \cos(x)$$



4 对候选方程进行偏微分处理

$$\frac{\partial}{\partial y}[f] = y + \sin(x) \frac{\Delta x}{\Delta y}$$

$$\frac{\partial y}{\partial x} \Big|_{f(x,y)} = \frac{\partial f}{\partial x} / \frac{\partial f}{\partial y}$$



$$1.37 \cdot \omega^2 + 3.29 \cdot \cos(\theta)$$

Lagrangian

$$2.71\alpha + 0.054\omega - 3.54\sin(\theta)$$

Equation of motion

$$(x - 77.72)^2 + (y - 106.48)^2$$

Circular manifold

$$\omega_1^2 + 0.32\omega_2^2 -$$

$$124.13\cos(\theta_1) - 46.82\cos(\theta_2) +$$

$$0.82\omega_1\omega_2\cos(\theta_1 - \theta_2)$$

Hamiltonian

哈密顿量、拉格朗日量

借助强大的计算能力自动从实验数据中提取物理定律

第 7 章 综合实验: AI for Science——自然规律和控制方程的符号回归提取算法研究

7.1 实验目的

1. 掌握符号回归的概念、原理和面临的挑战,了解目前在材料领域常用的符号回归算法 SISSO 的设计思路。
2. 学会对算法中的超参数调优,对算法框架中不同模块的设计根据需求进行调整,分析算法收敛性。
3. 自主构建符号回归算法实现纳米粒子生长动力学中生长级数方程的提取。