Unveiling Metal Organization in Single-Atom Catalysts through Advanced Microscopy and Machine Learning

May 13-17, 2024

Machine Learning Modalities for Materials Science

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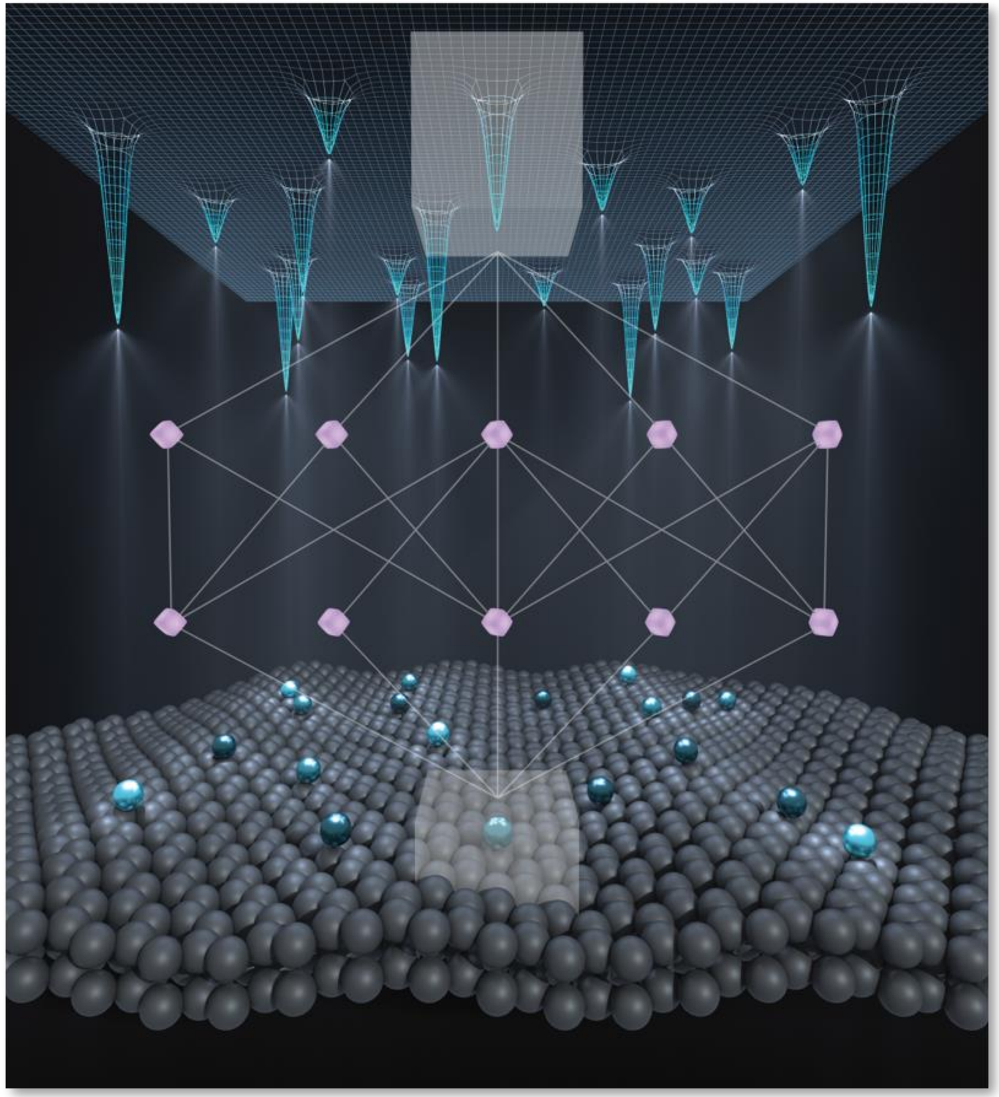
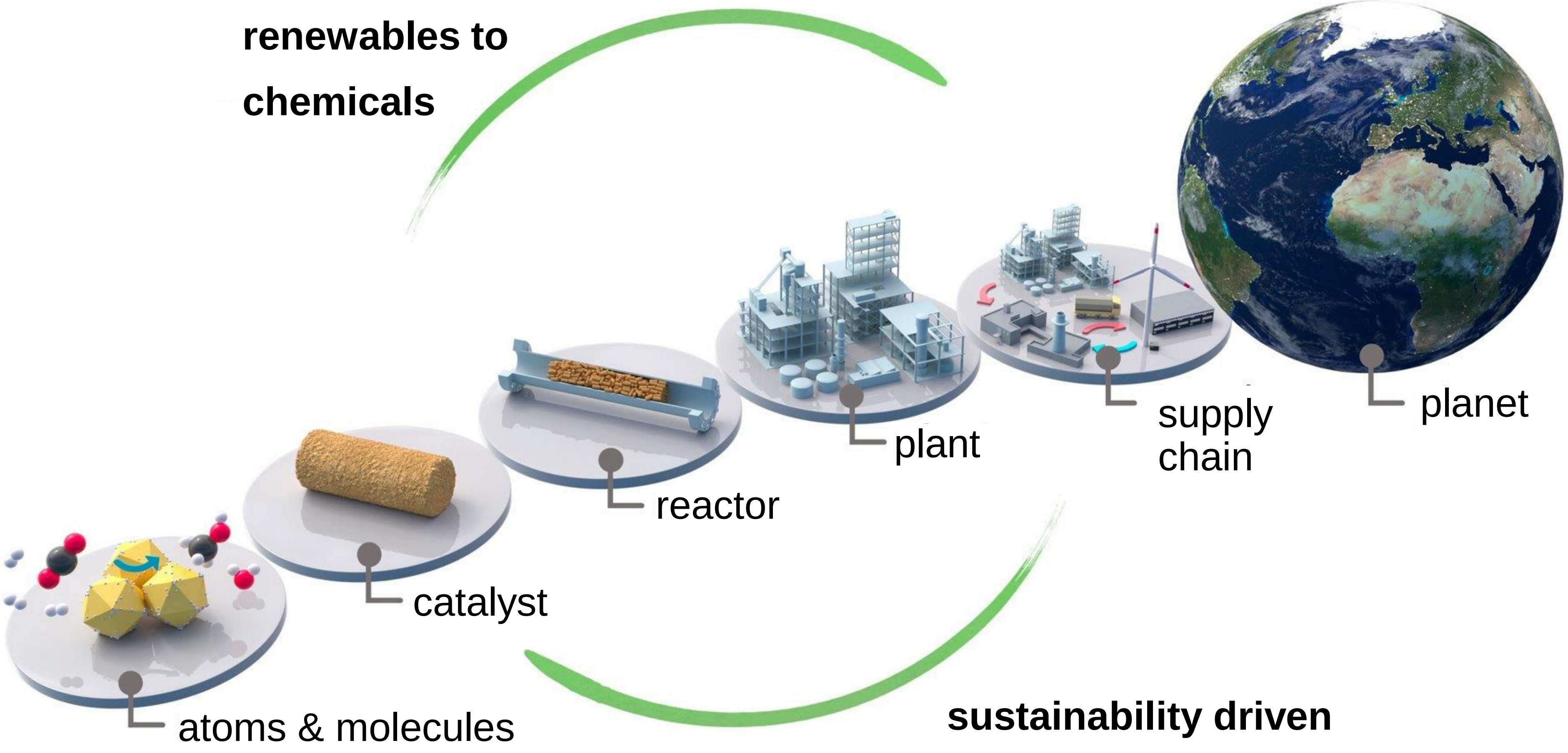


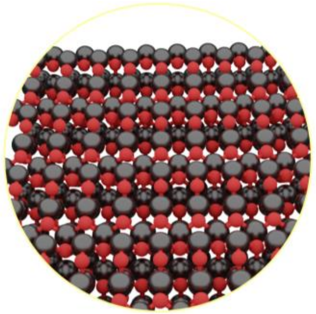
Sustainable catalysis



Angew. Chem. Int. Ed. **2024**, e202318676

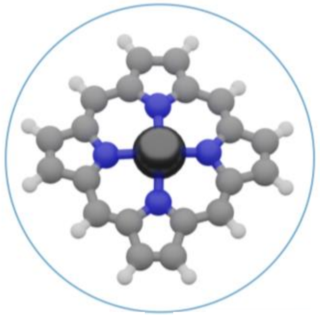
Sustainable catalysis

Heterogeneous



High amounts of metal

Risk of leaching



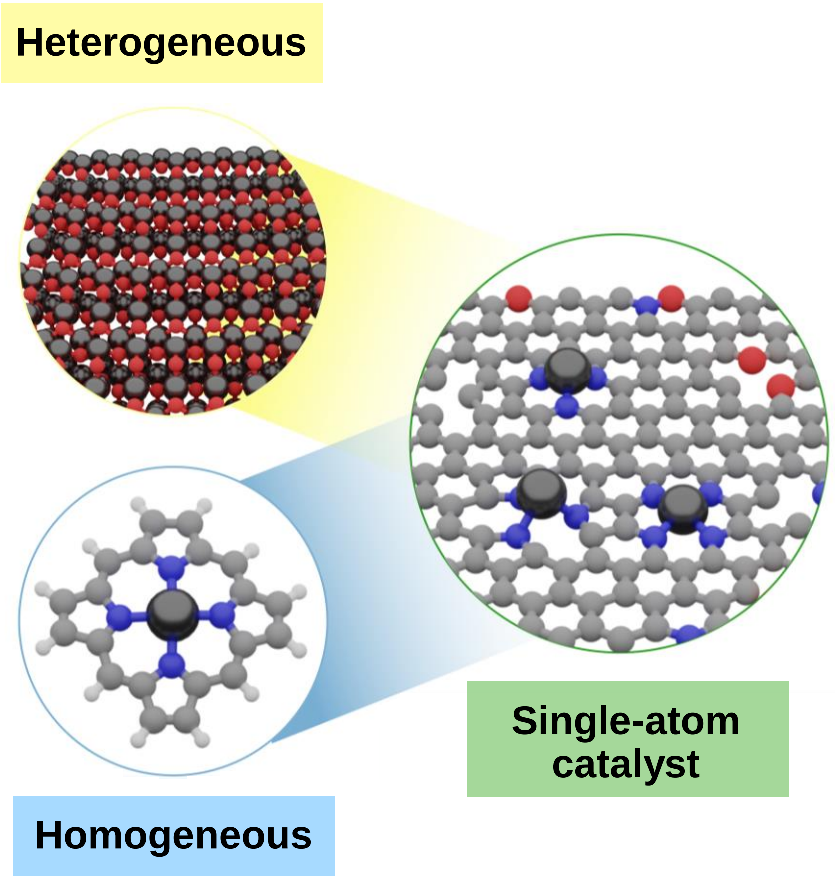
Catalyst separation

Waste generation

Homogeneous

Nature Reviews Chemistry, **2018**, *2*(6), 65-81 | Nature Chemistry, **2011**, *3*(8), 634-641

Sustainable catalysis

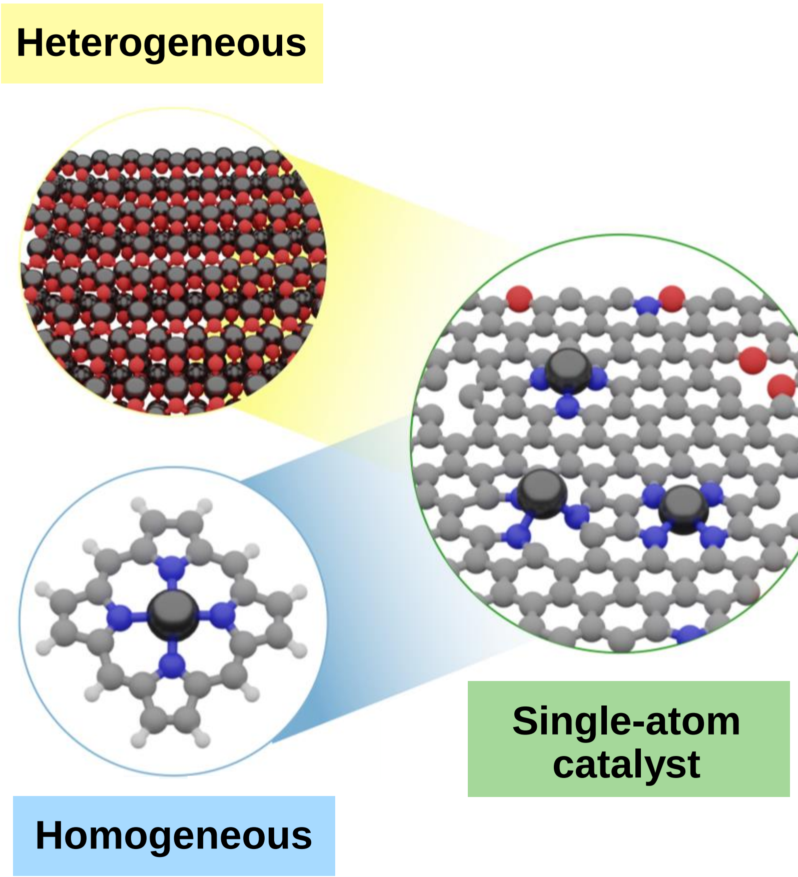


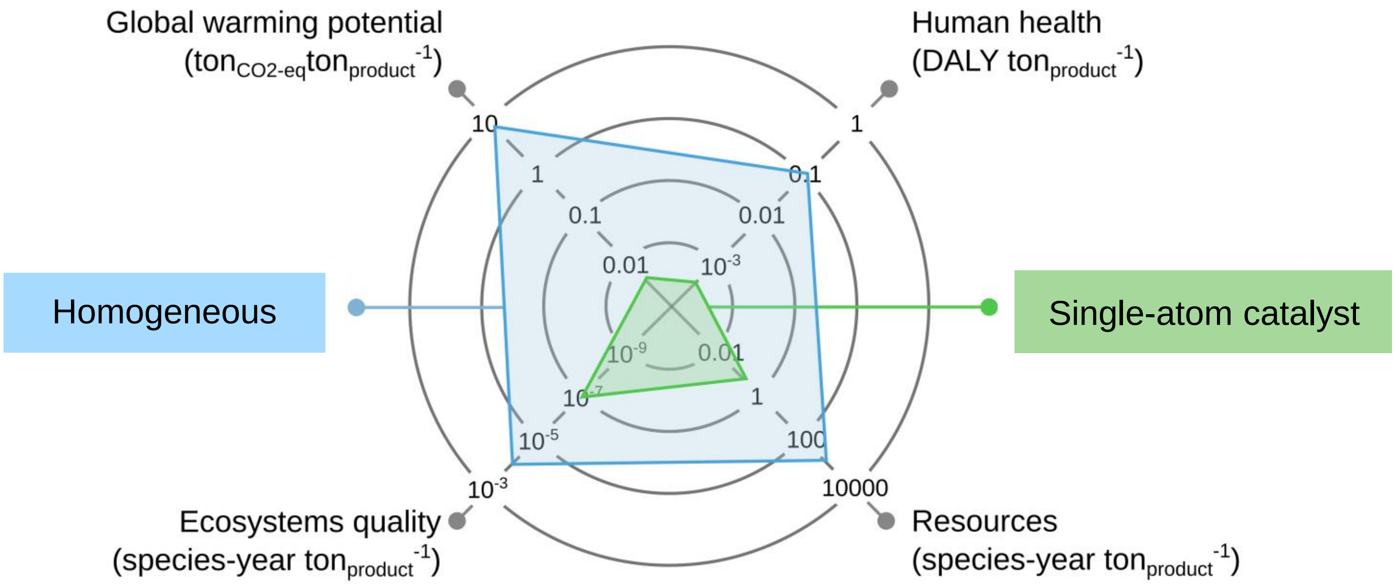
Unified theory in Catalysis

Bridging the best of heterogeneous and homogeneous catalysis

Nature Reviews Chemistry, **2018**, *2*(6), 65-81 | Nature Chemistry, **2011**, *3*(8), 634-641

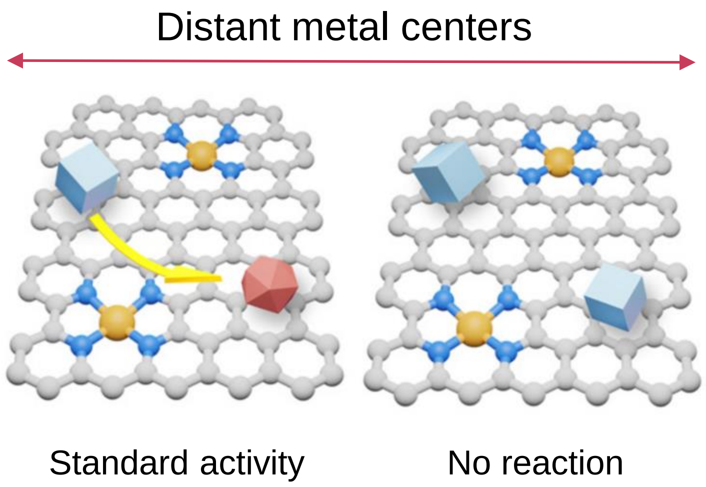
Sustainable catalysis



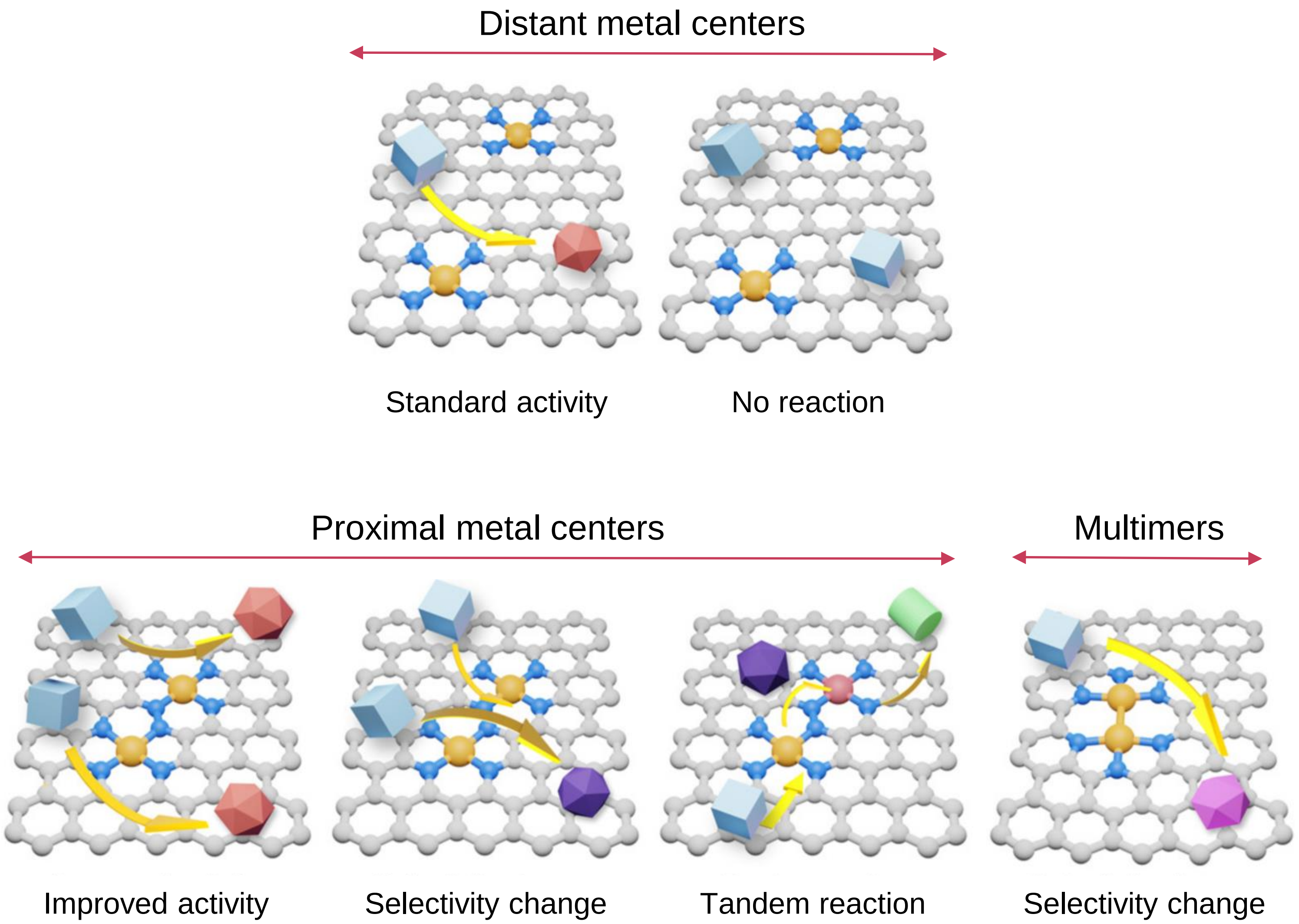


Green Chem, **2022**, *24*, 6879-6888

Ultra-high density single atom catalysts

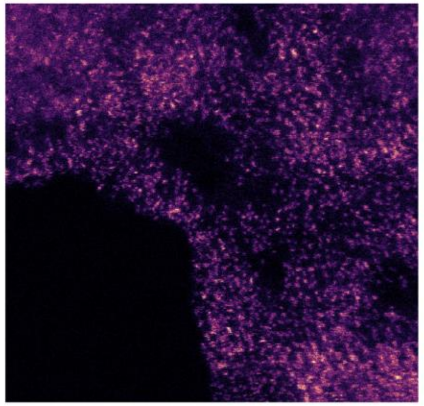


Ultra-high density single atom catalysts



Catalyst characterization

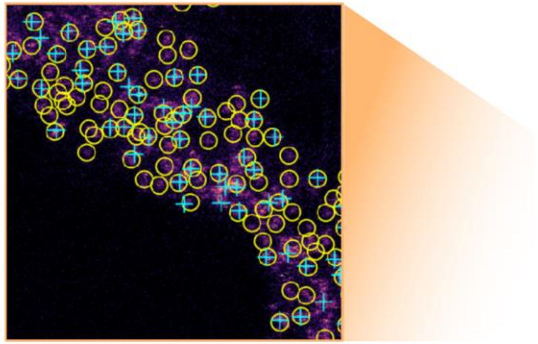
(S)TEM



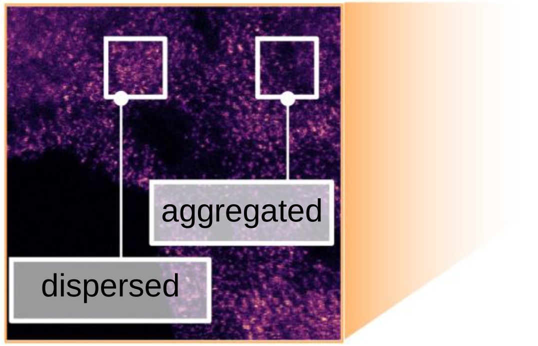
JACS, **2022**, *144*(18), 8018-8029 | Nature Reviews Methods Primers, **2022**, *2*(1), 11.

Catalyst characterization

Conventional analysis

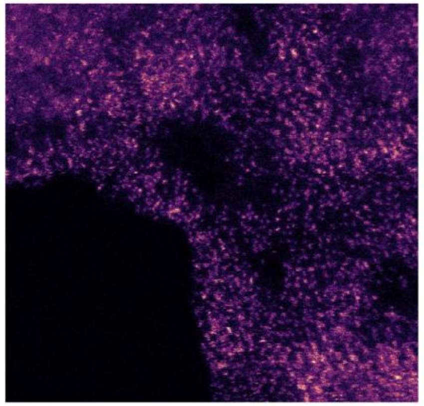


Manual atom
detection



Qualitative
dispersion

(S)TEM



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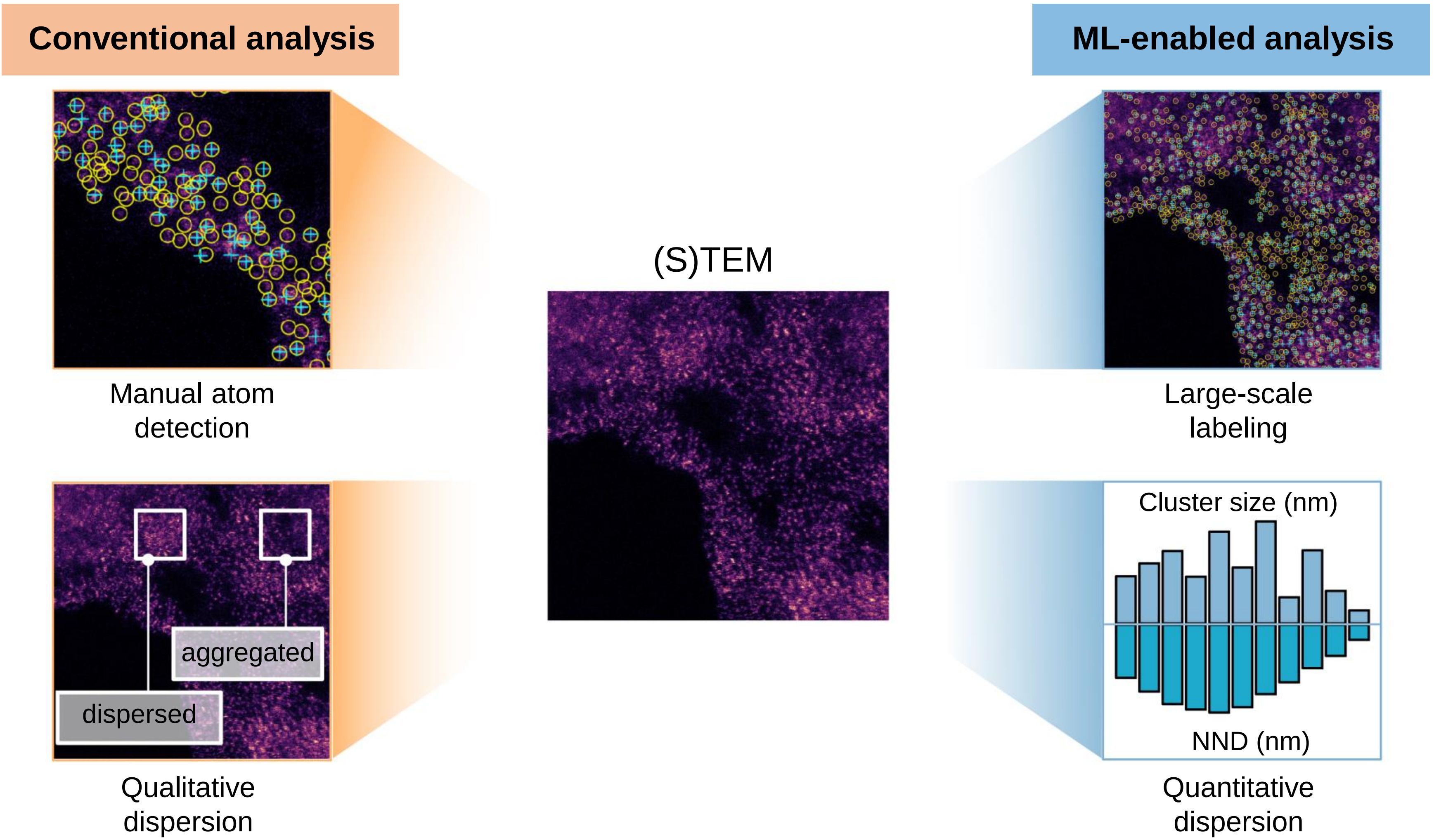
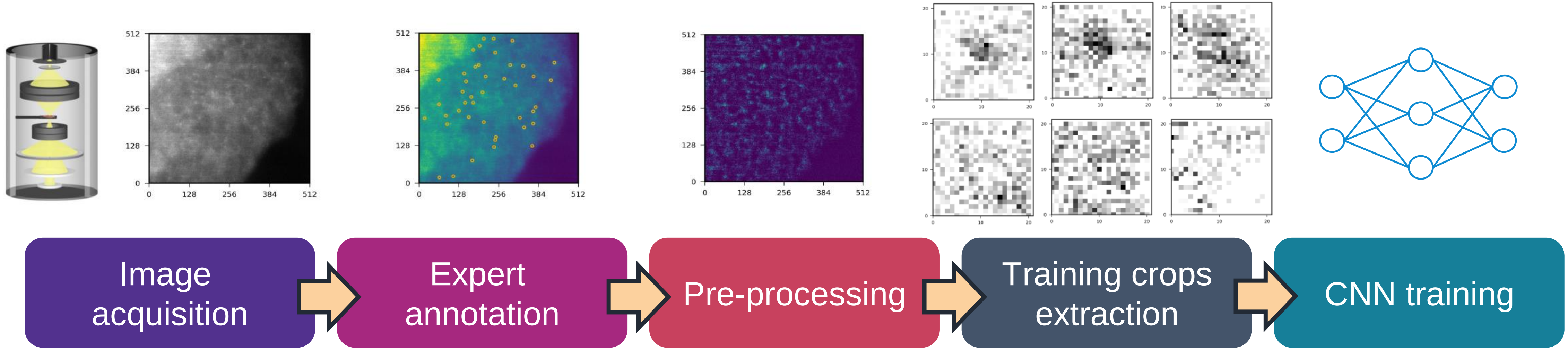
Catalyst characterization



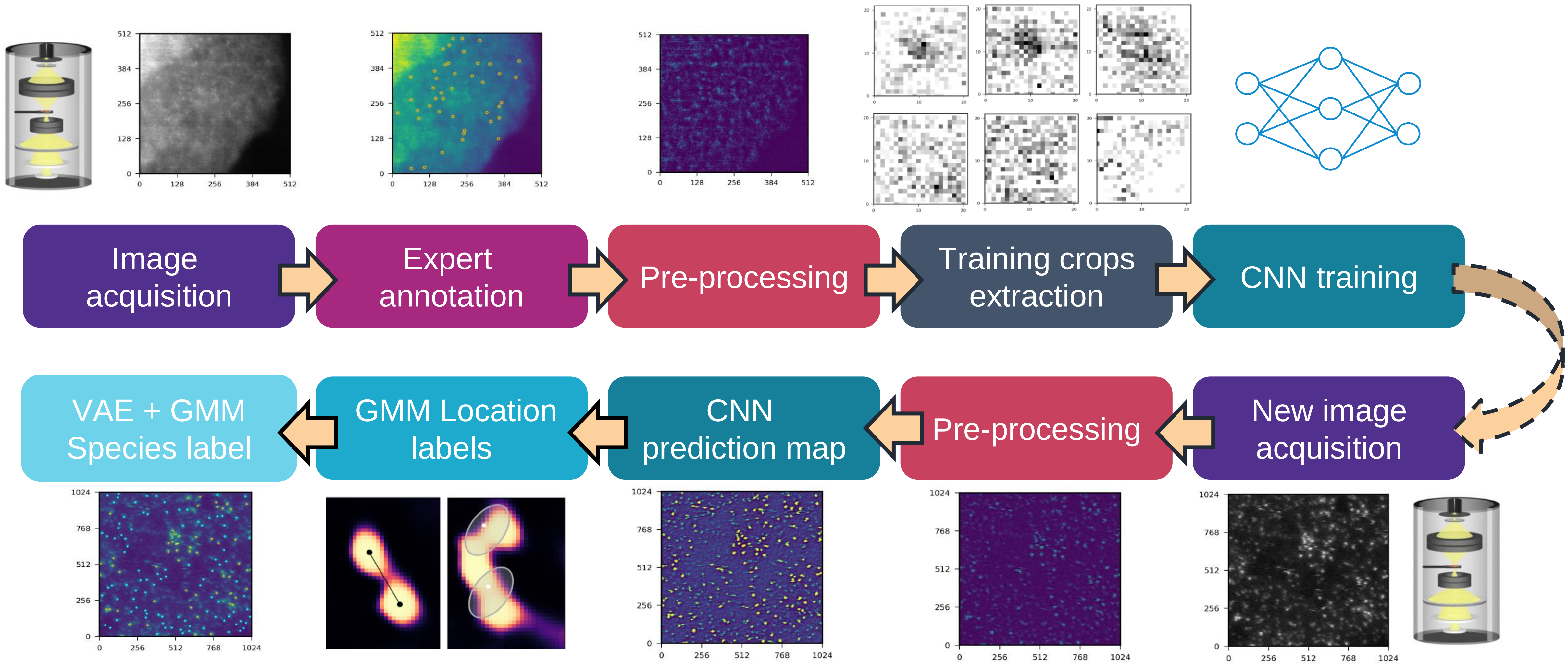
JACS, **2022**, *144*(18), 8018-8029 | Nature Reviews Methods Primers, **2022**, *2*(1), 11.

Automated SAC STEM Image Analysis Workflow

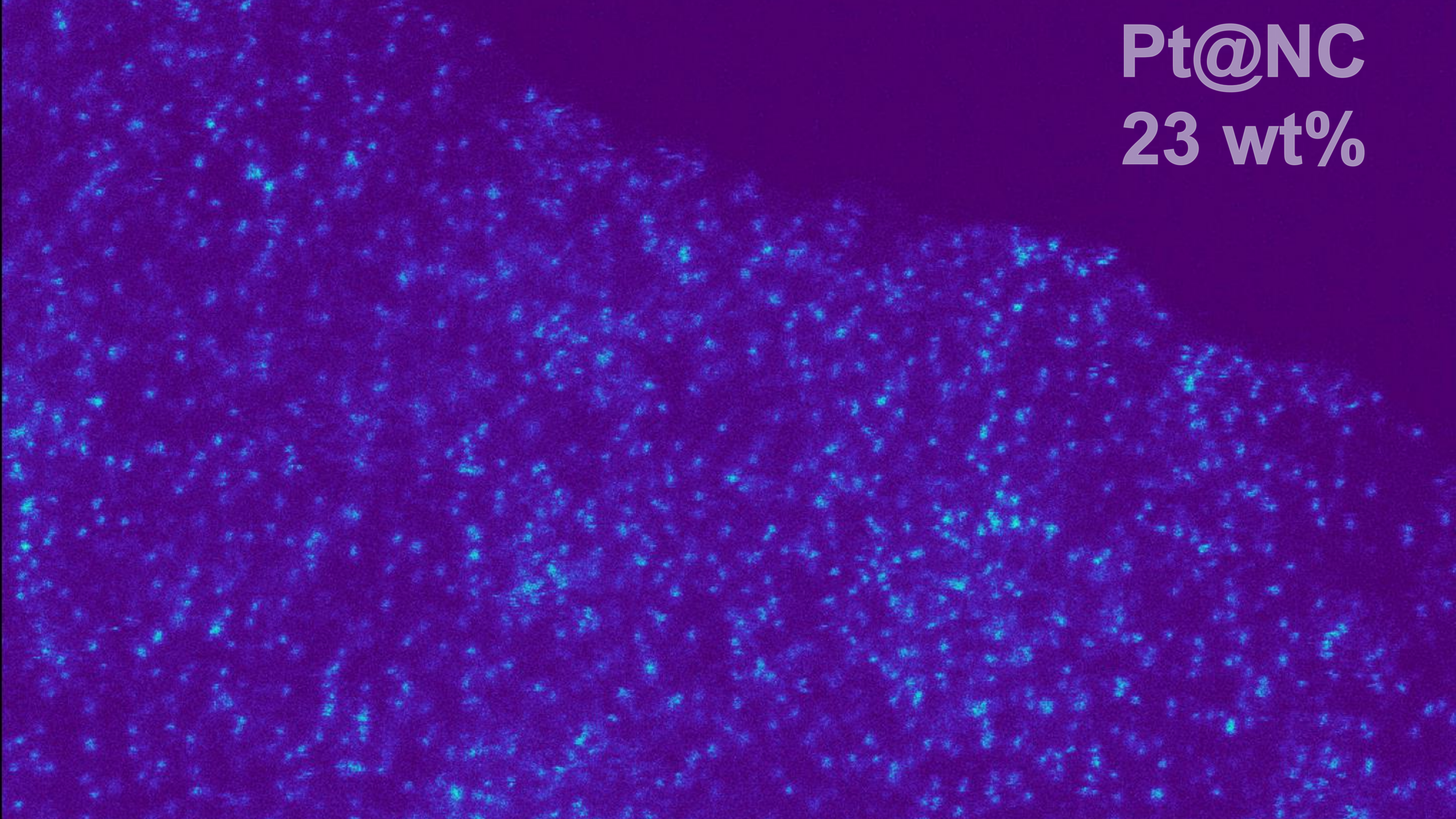


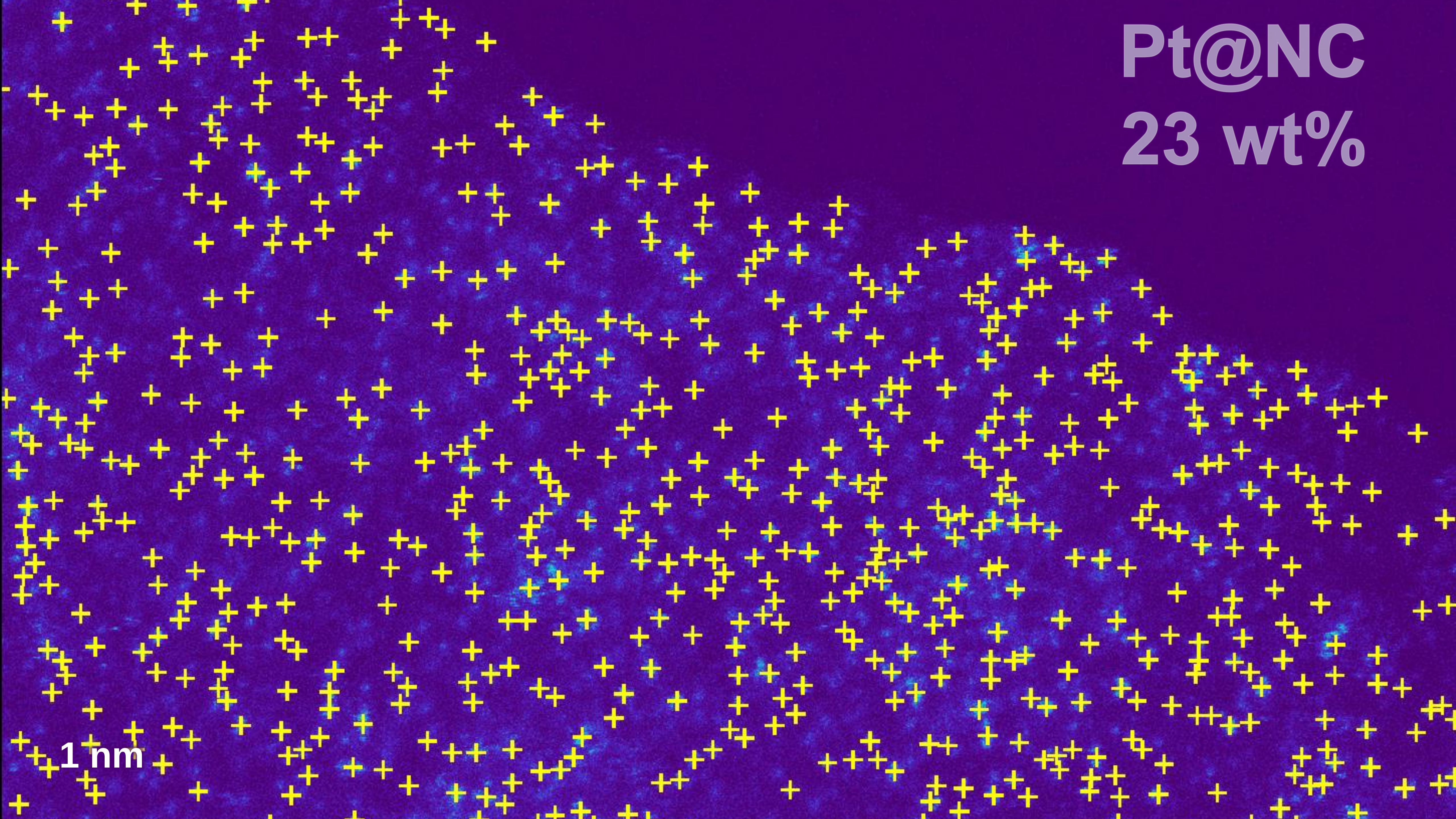
Advanced Materials, **2024**, *36*(5), 2307991

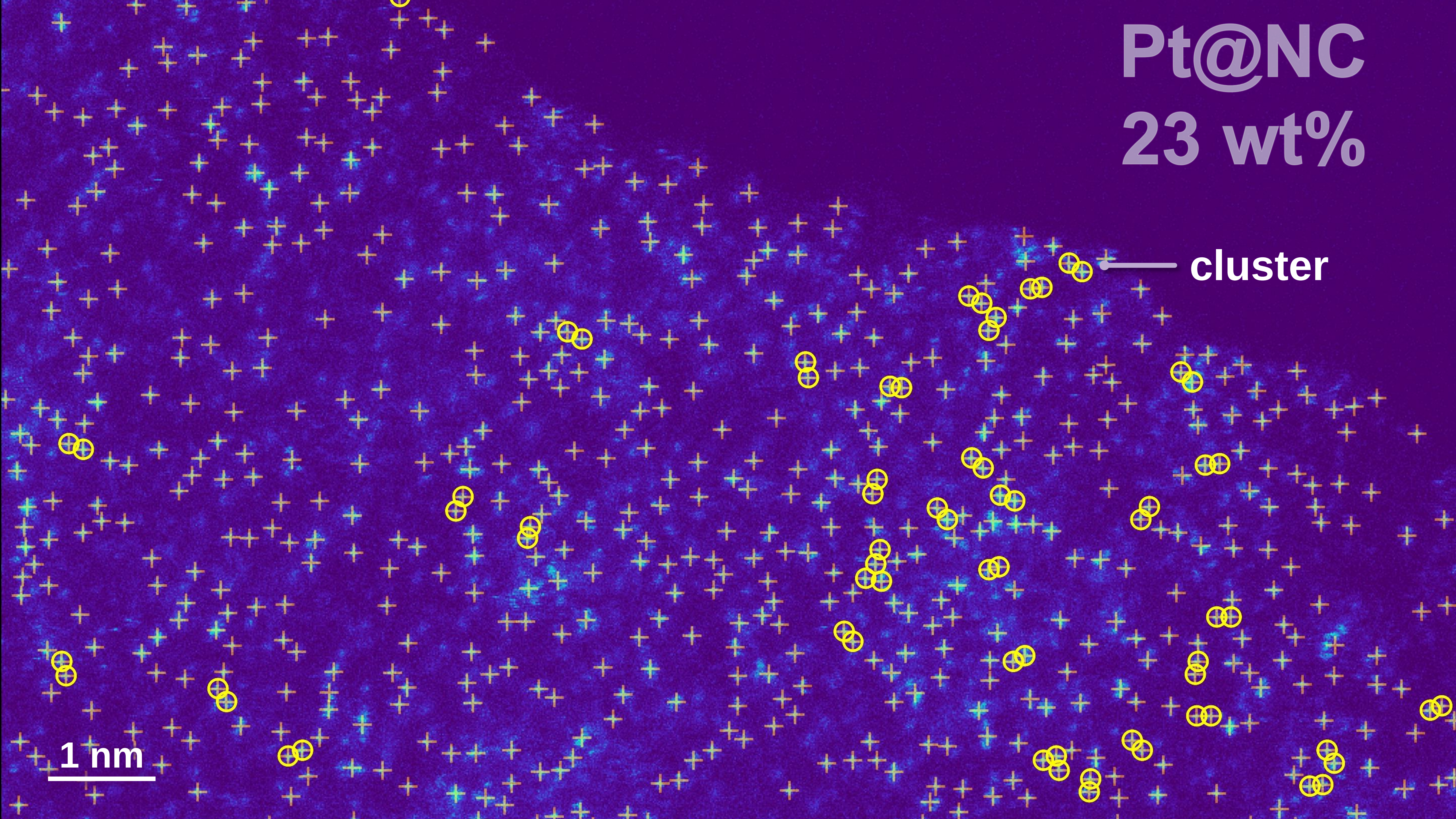
Automated SAC STEM Image Analysis Workflow

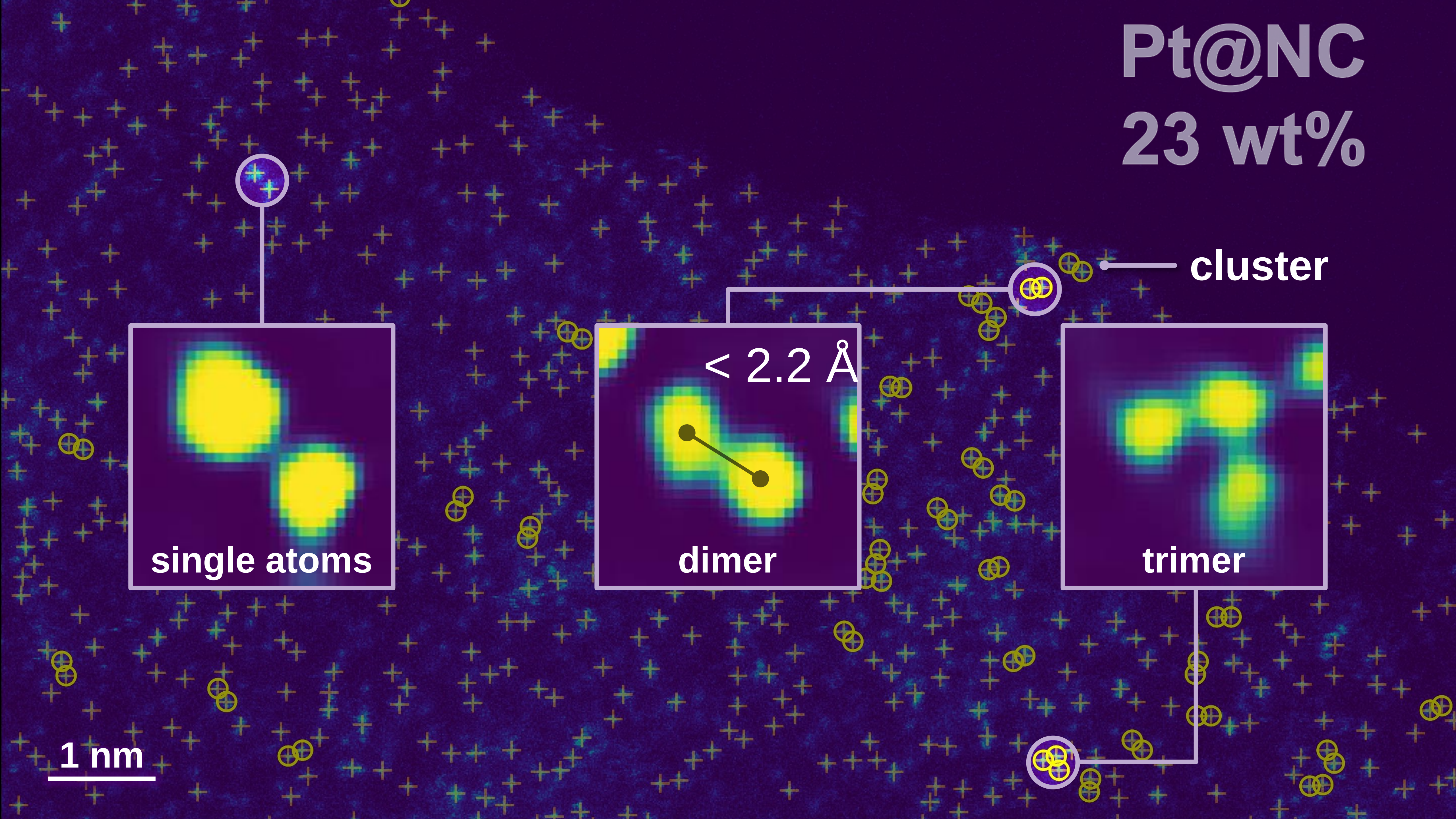


Advanced Materials, **2024**, *36*(5), 2307991


Pt@NC
23 wt%


Pt@NC
23 wt%
1 nm


Pt@NC
23 wt%
cluster
1 nm

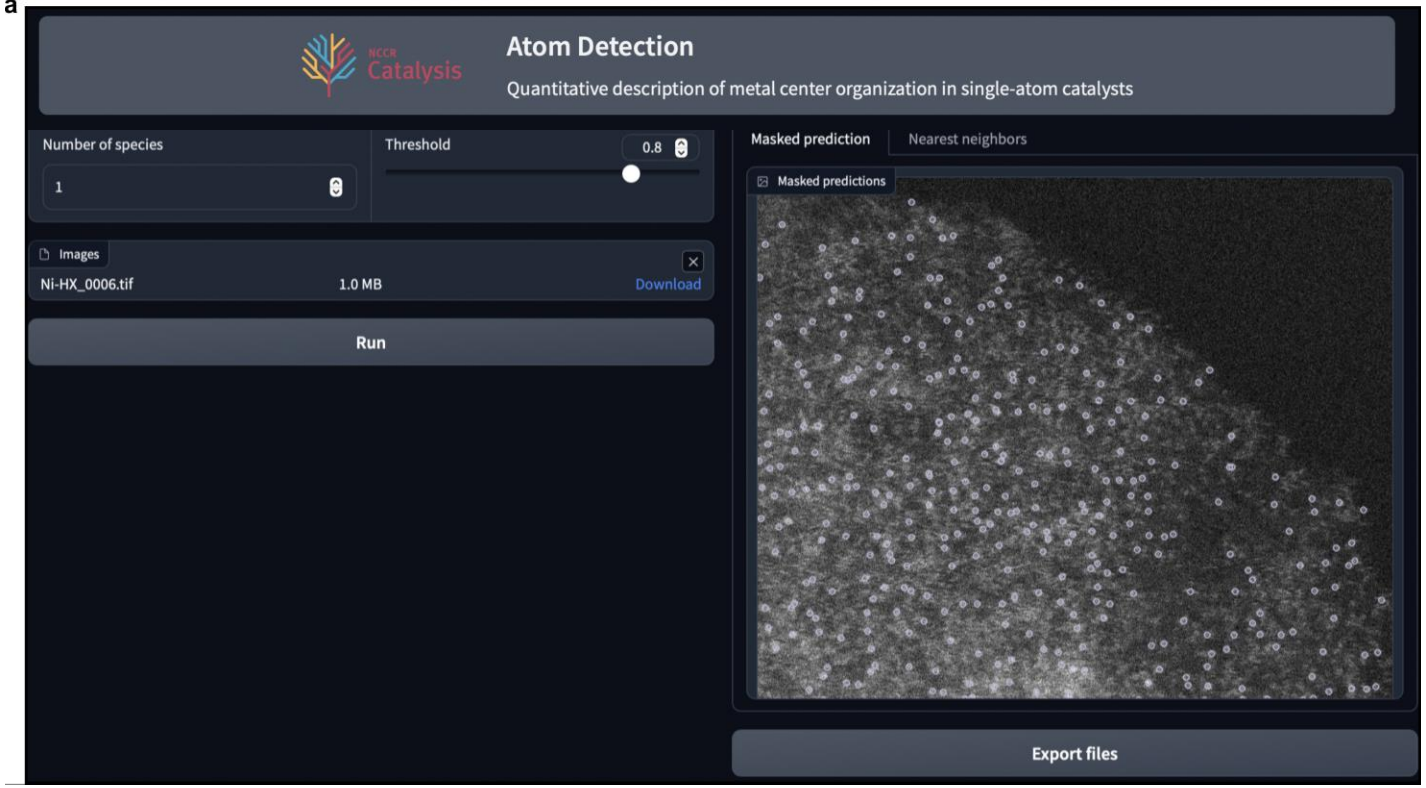

Pt@NC
23 wt%
cluster
< 2.2 Å
single atoms
dimer
trimer
1 nm

Digital tools for our community

Stem Atoms

Project ID: 223

a



Efficient and automated analysis

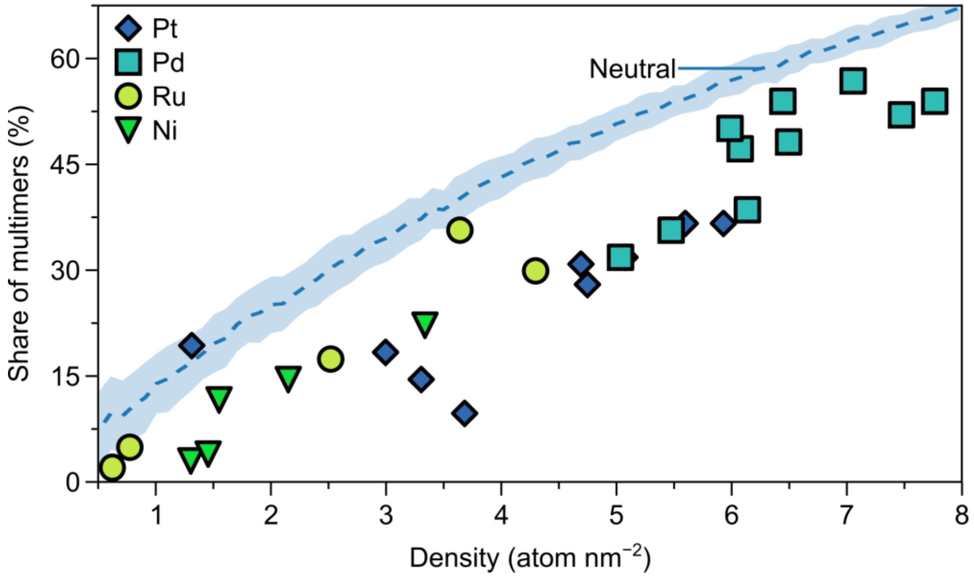
Standardized and reproducible

General and transferable

Open-access

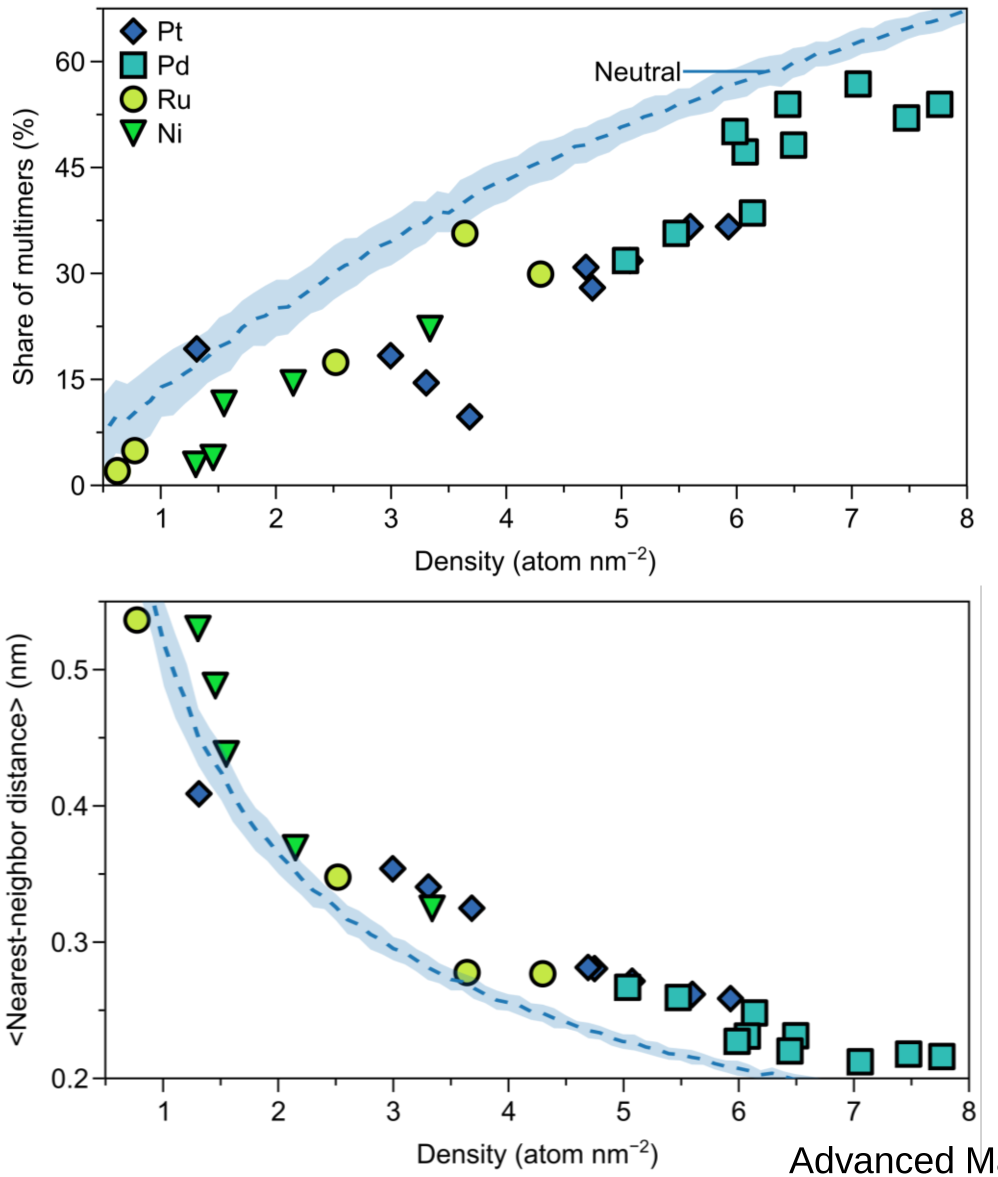
Advanced Materials, **2024**, *36*(5), 2307991

Digital tools for novel insights



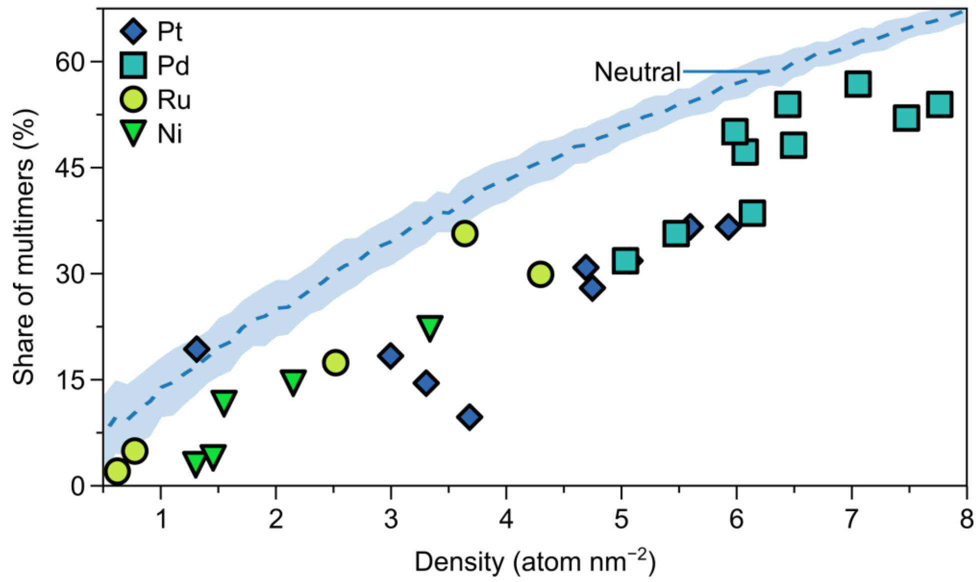
Advanced Materials, **2024**, *36*(5), 2307991

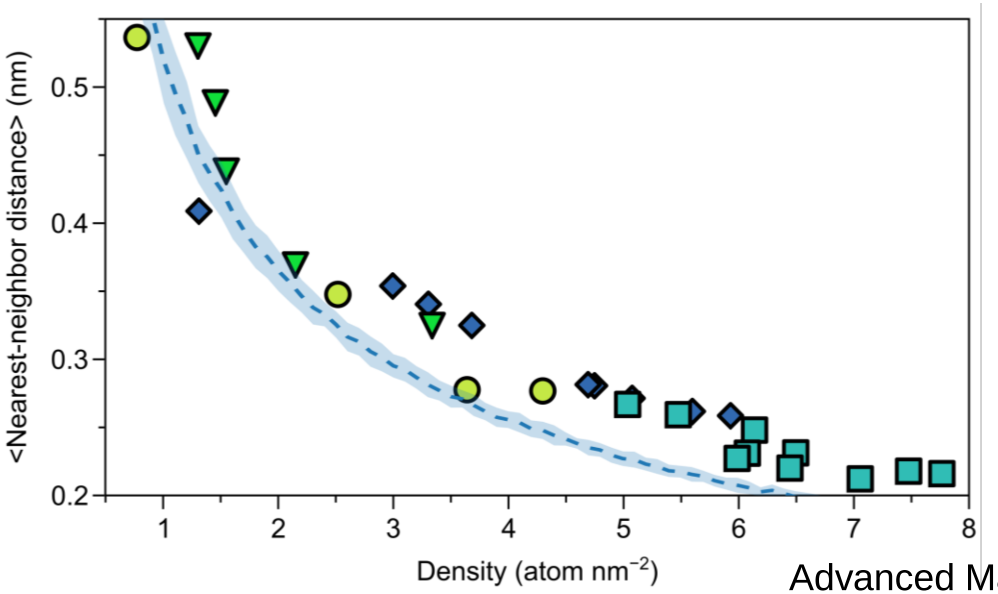
Digital tools for novel insights

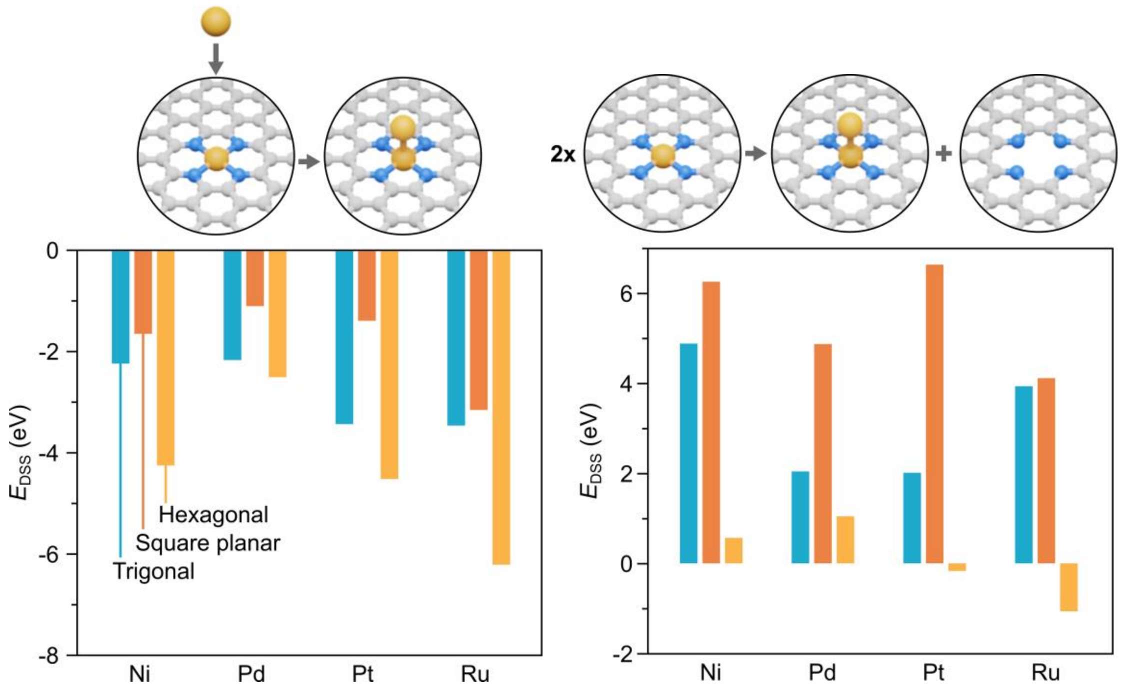


Advanced Materials, **2024**, *36*(5), 2307991

Digital tools for novel insights

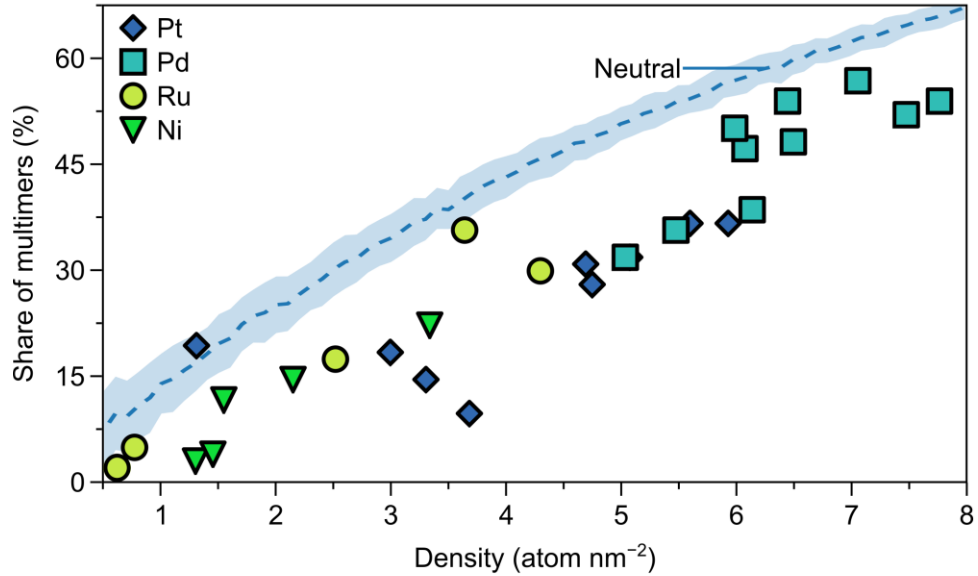


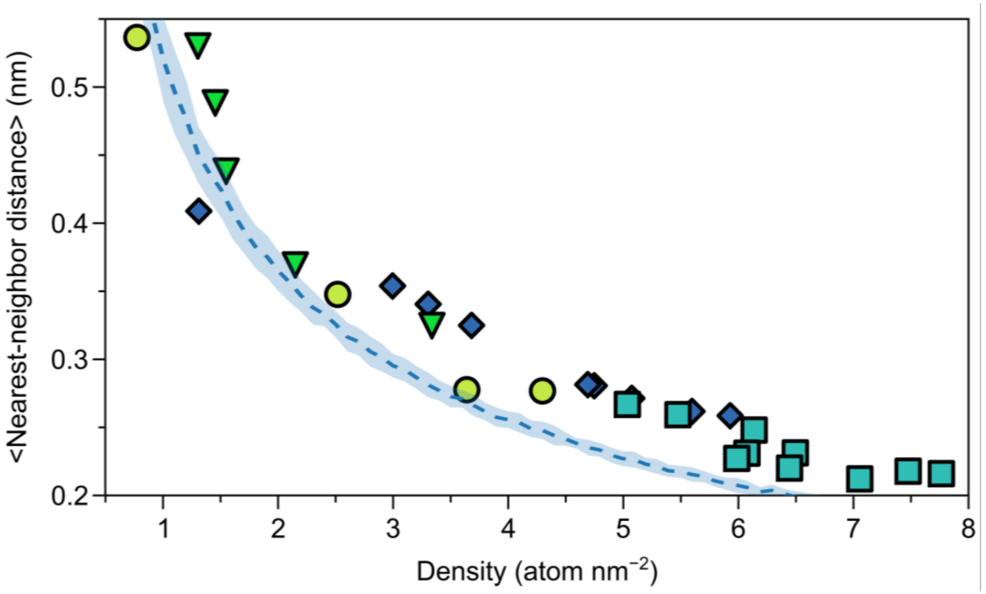


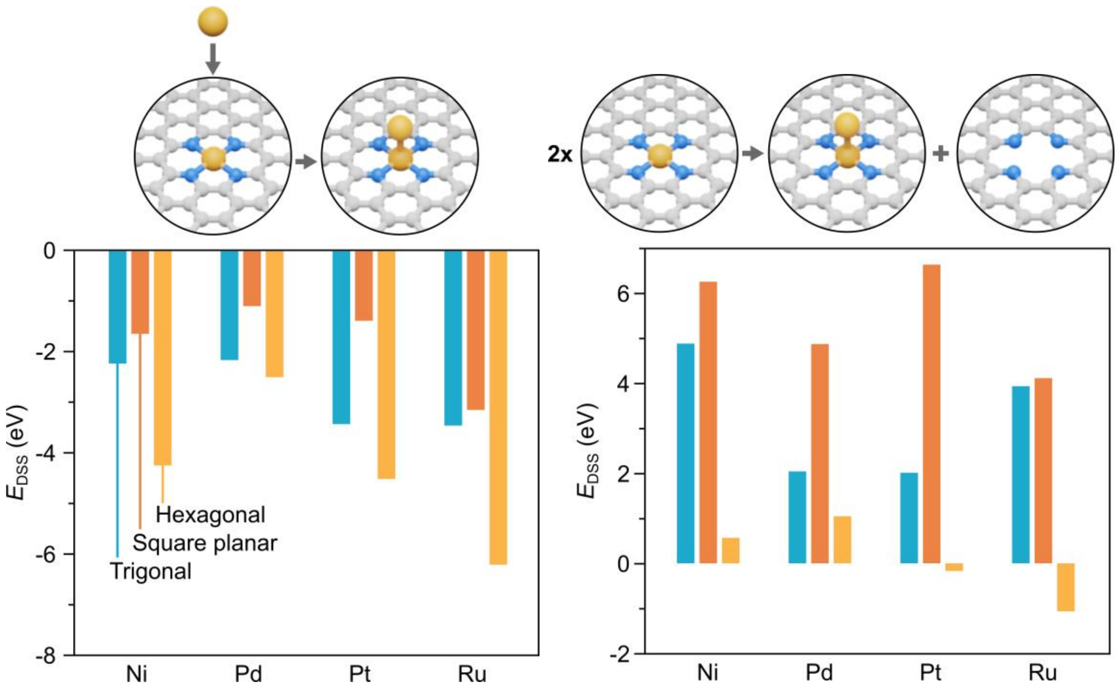


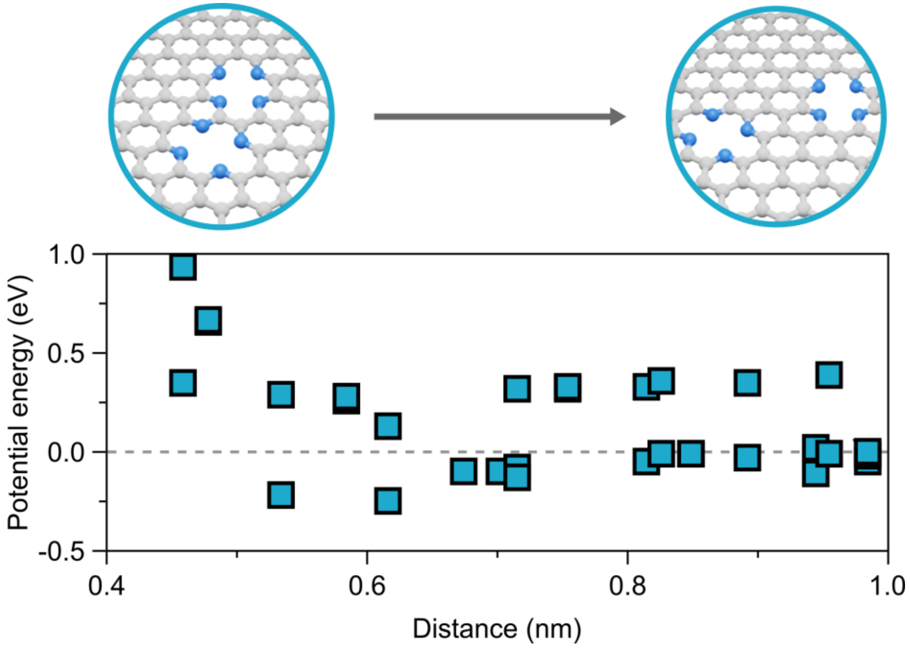
Advanced Materials, **2024**, *36*(5), 2307991

Digital tools for novel insights

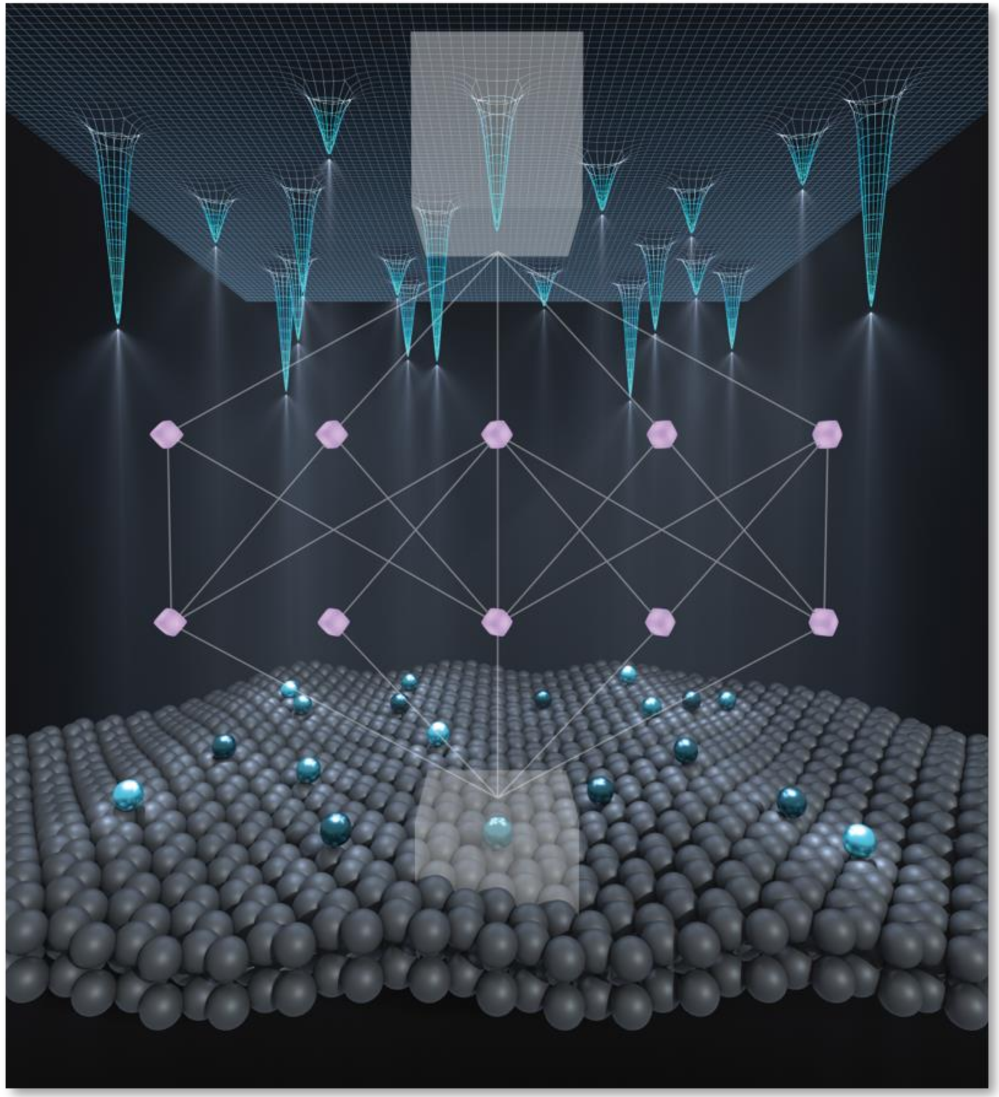








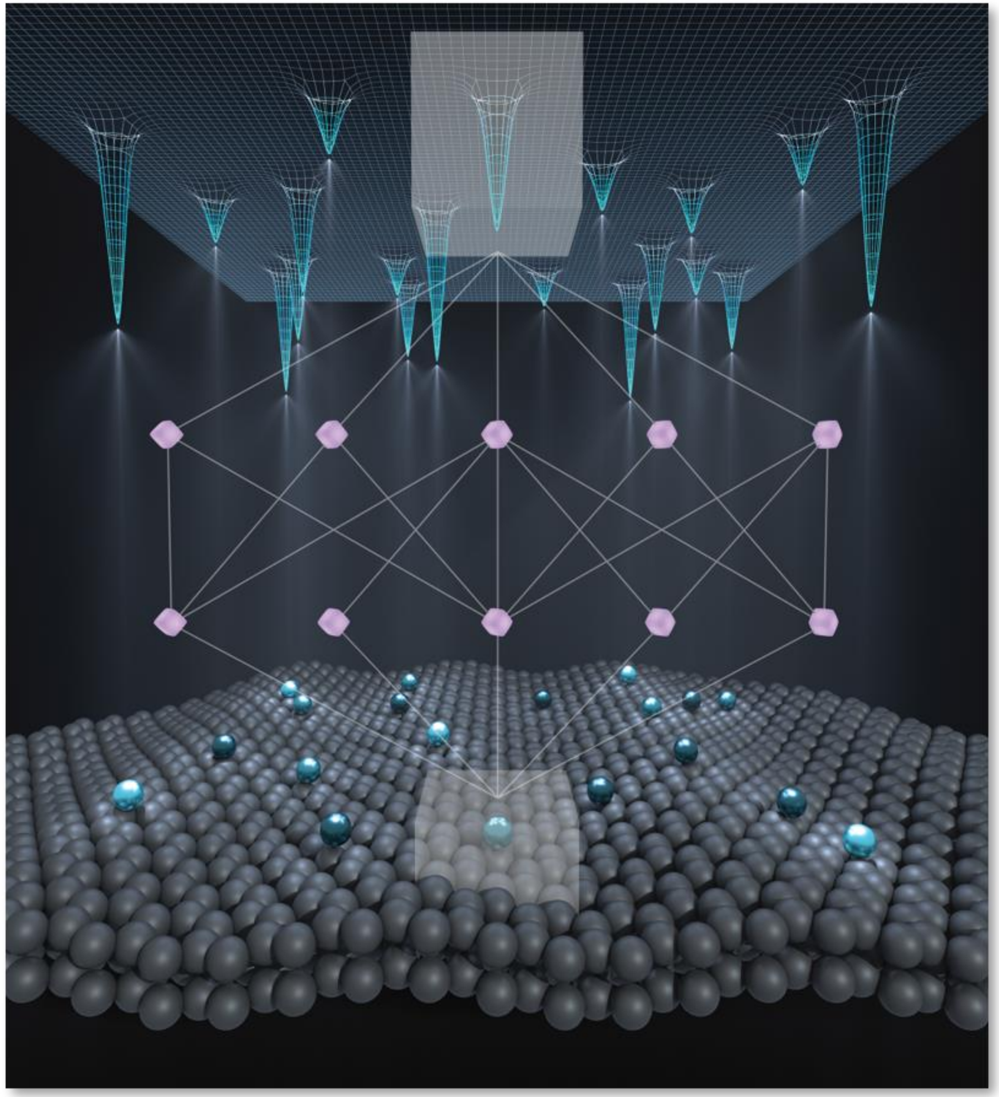
Conclusions



Beyond the isolated atom limit

Quantitative insights of metal distribution

Conclusions



Beyond the isolated atom limit

Quantitative insights of metal distribution

Future prospects

Standardization of analysis methodologies

Integrate pipeline to other techniques

ICIQ
Institut Català d'Investigació Química

BSC Barcelona Supercomputing Center
Centro Nacional de Supercomputación

ETH zürich

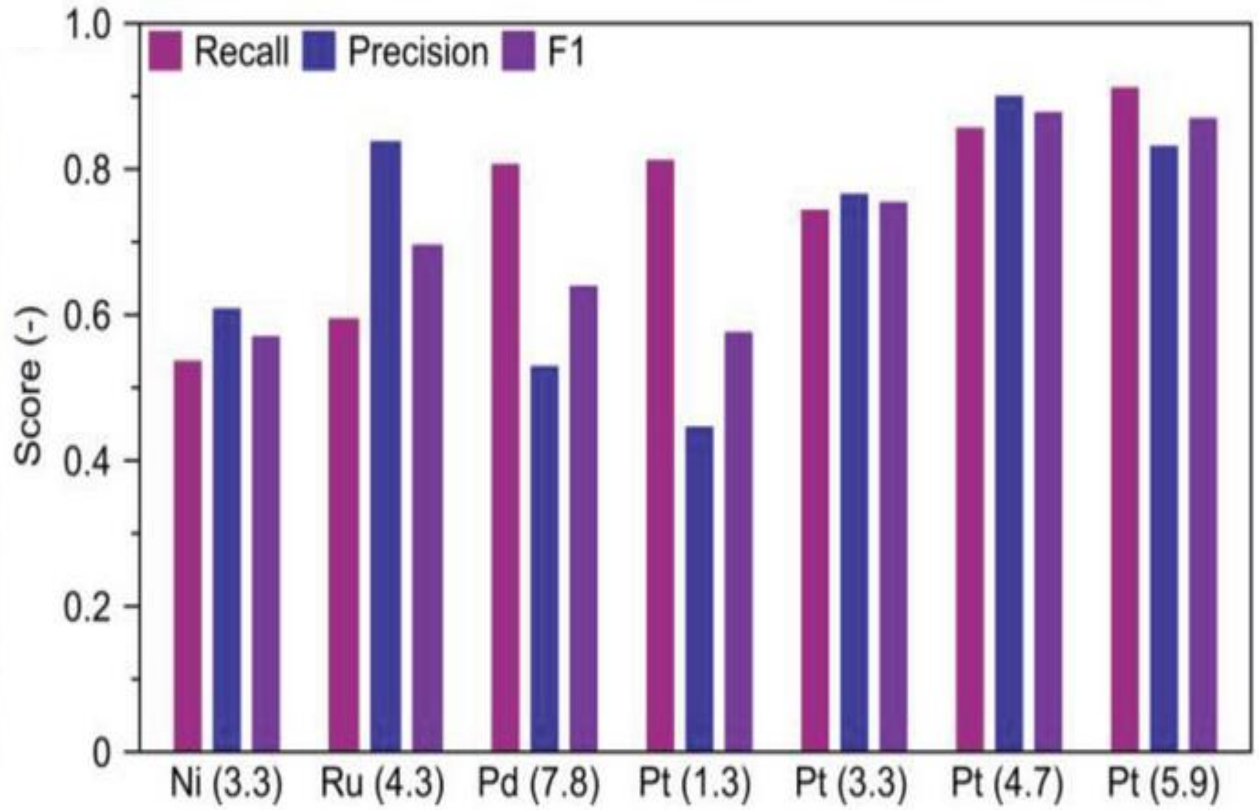
cost
EUROPEAN COOPERATION IN SCIENCE & TECHNOLOGY

NCCR Catalysis

ML4MS

Thank you!

Model Performance



$$Precision = \frac{TP}{TP + FP} \qquad Recall = \frac{TP}{TP + FN}$$

$$Accuracy = \frac{TP + TN}{TP + FP + FN + TN}$$

$$F1\ Score = 2 \times \frac{Precision \times Recall}{Precision + Recall}$$

Performance increases with higher atomic number

Less tendency to false positives; but inherent challenge in lighter atoms (also evident to domain experts)

Additional information on the pipeline

Training data points: more than 8000 metal centers detected by the human-expert.

Limitations: ground truth is subject to human bias in visual perception.

Next steps in the use of the supervised approach: platform to crowdsource annotations to standardize and quantify the uncertainty associated with the predictions made by the model.