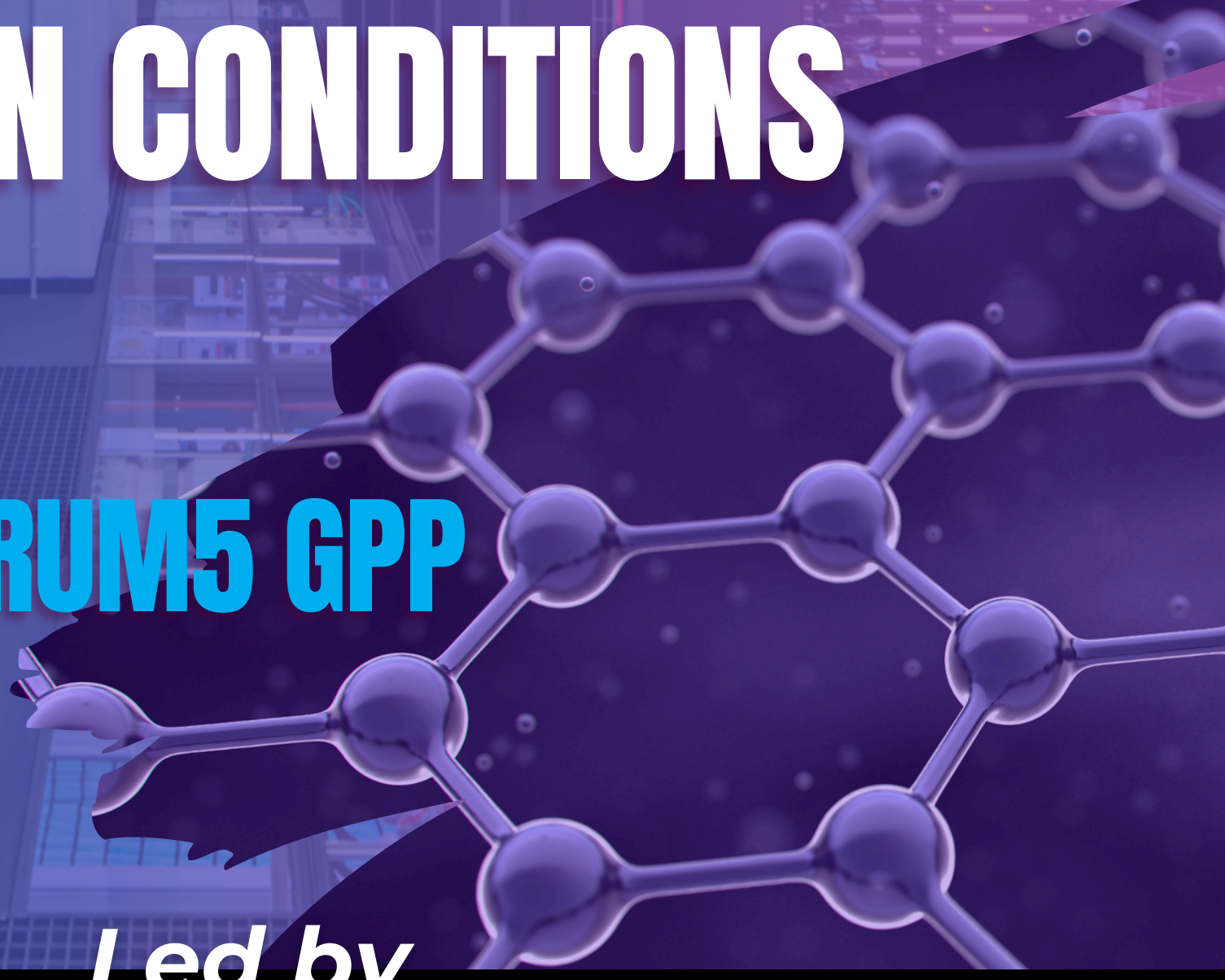
PREDICTING STABLE STATES OF SILVER NANOPARTICLES UNDER REACTION CONDITIONS

MARENOSTRUM5 GPP



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1 HOW DO CATALYSTS EVOLVE DURING REACTIONS?

47
Ag
Silver
107.8682

Transition metals are essential components of many **catalytic and energy technologies**

Their **performance** in such applications is strongly **influenced by the surrounding environment**

In oxygen-rich conditions, catalysts can undergo **significant structural changes through oxidation**

Understanding and modeling these transformations is crucial for the **design of more efficient catalytic materials**

WHY IS THE CATALYST DESIGN SO CHALLENGING? 2

Describing the oxidation behaviour of metal catalysts is **not a trivial task, both experimentally and computationally**

The major difficulty lies in obtaining **accurate structural models** of the catalyst **before and after oxidation**

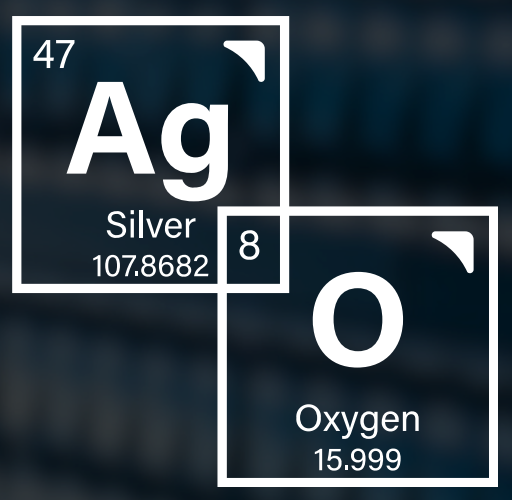
Adressing these challenges requires the **combination of different advanced simulation techniques**

Insights gained from **simple systems** can be **extended** to increasingly **realistic catalytic materials**

3 HPC-POWERED MODELLING OF SILVER NANOPARTICLES

High performance computing enabled **extensive Grand Canonical simulations** of silver substrates

These thousands of simulations addressed **systems ranging from extended surfaces to nanoparticles** with hundreds of Ag and O atoms



Computational power was crucial for the **Quantum Mechanical calculations used to validate the models**

This made it possible to build **high-quality datasets** and explore larger, more realistic catalytic systems

WHAT CAN WE LEARN FROM THE SIMULATIONS? 4

The simulations successfully **reproduced oxidized surface strucutures** reported in the literature, **validating the protocol**

They also provided **new insights** into oxidation, **revealing stable oxidized structures** for silver nanoparticles of different shapes

Active learning strategies further **improved predictive accuracy and identification of stable oxidized configurations**

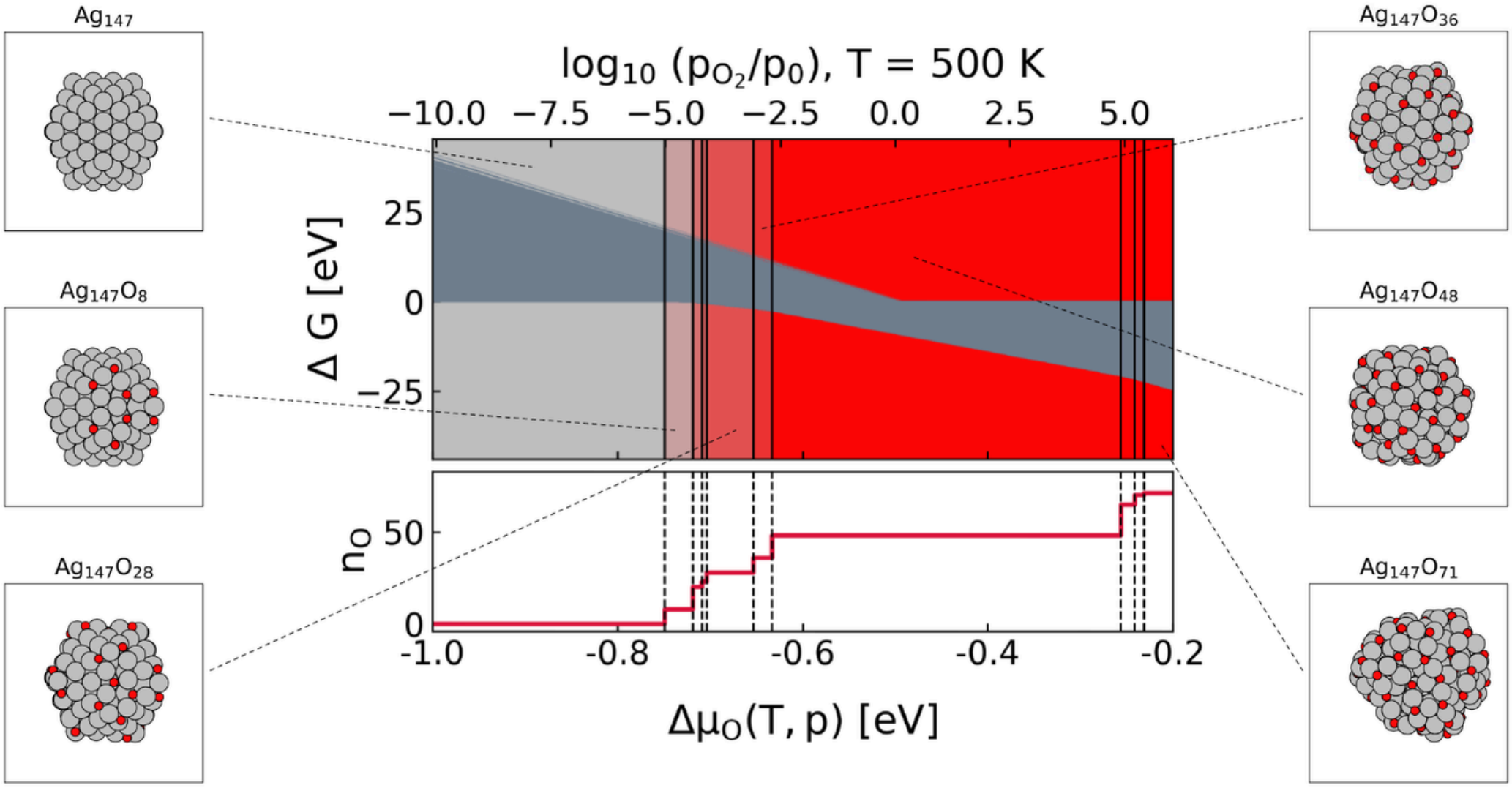


Figure: Phase diagram and most relevant structures for an icosahedrall Ag_{147} nanoparticle.

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