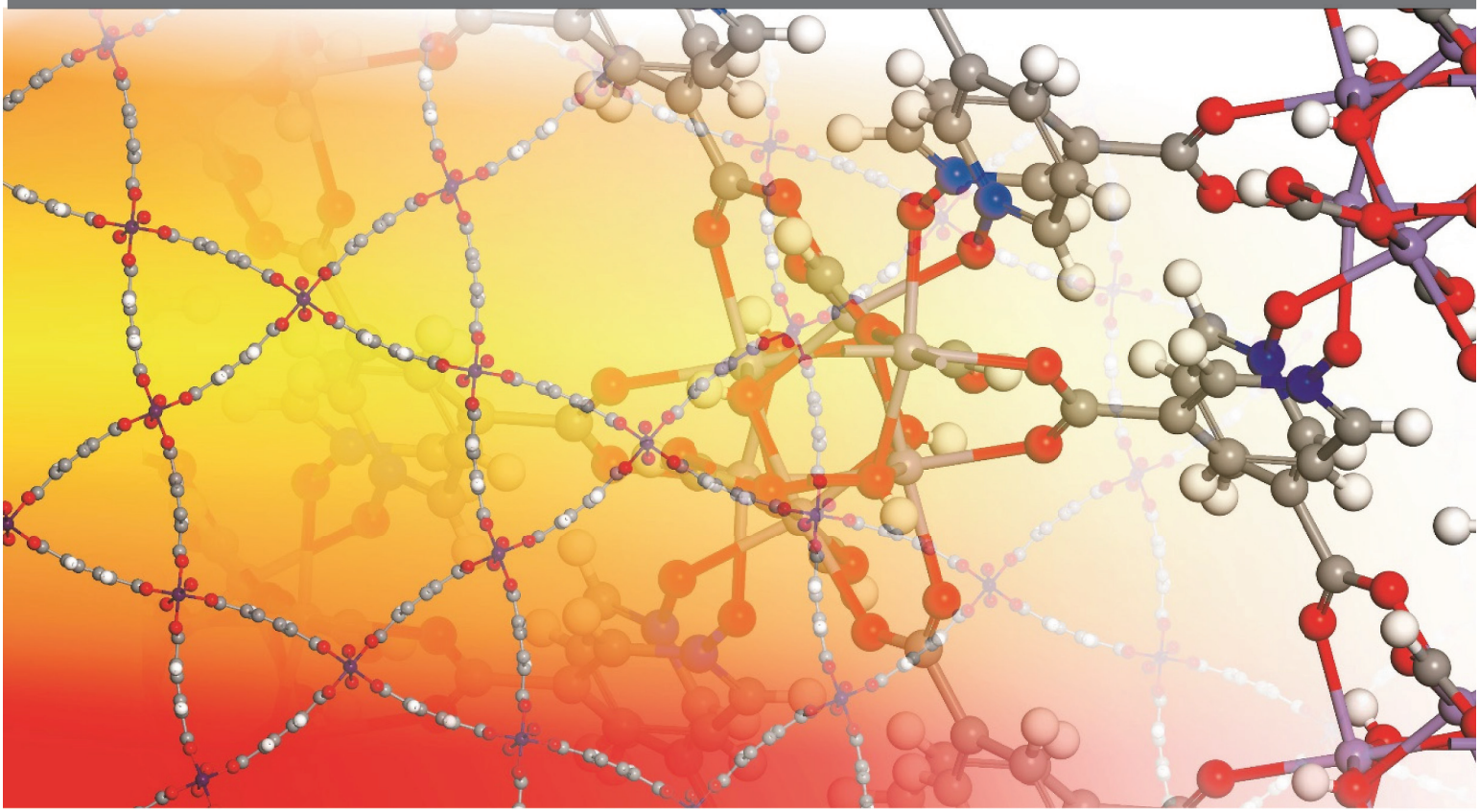
COMPUTATIONAL MATERIALS ENGINEERING TEAM



NETL

NATIONAL ENERGY TECHNOLOGY LABORATORY

BACKGROUND

The U.S. Department of Energy's (DOE) National Energy Technology Laboratory's (NETL) Computational Science & Engineering (CSE) Directorate is recognized for its ability to develop science-based simulation models, mathematical methods and algorithms, and software tools to address the technical barriers in the development of next-generation energy technologies. This competency works in collaboration with other capabilities at NETL to generate information and scientific understanding beyond the reach of experiments alone through the integration of experimental information with computational sciences across different time and length scales. The CSE Directorate is organized into three teams: 1) Computational Materials Engineering, 2) Computational Device Engineering, and 3) Data Analytics teams that collectively maintain NETL's Computational Science and Engineering competency.

COMPUTATIONAL MATERIALS ENGINEERING TEAM

The Computational Materials Engineering (CME) Team maintains expertise in the modeling of materials at the atomic, molecular, and meso scales, which enables a fundamental understanding of materials behavior and provides insight into subsequent materials development opportunities and optimization strategies. The team uses combinations of these general approaches, in conjunction with experimental results, to develop new materials or conceptual processes with improved reliability. These processes allow the CME Team to assess the performance of emerging new materials in the context of new energy technologies and to identify ways to improve materials efficiency, performance and cost.

By employing highly accurate computational approaches, including first principles quantum mechanics calculations, classical and quantum molecular dynamics, Monte Carlo simulations, microkinetic modeling, and mesoscale modeling, the CME Team is able to characterize the materials properties involved in diverse applications of interest. These include catalysts and electrocatalysts, solid and liquid membranes for gas capture and separation, oxygen carrier materials, materials for solid oxide fuel cell applications, and novel nanostructured materials for energy conversion and the development of gas sensors.

Additionally, the team uses advanced computational methods, including high-throughput computational screening, to design materials or novel alloy compositions with controlled properties. These methods allow researchers to evaluate materials' thermomechanical and microstructure evolution under heat or electromagnetic treatments, optimize performances under diverse process conditions, and assess performance-to-cost ratio.

CAPABILITIES

To address the range of time and length scales involved in developing new materials with the optimized performances required by current energy technologies, the CME Team employs capabilities in four areas:

Quantum mechanics-based simulation capabilities. The team uses various ab initio molecular orbital packages (Gaussian, Molpro, Q-Chem, DMol) for describing the structural and electronic properties of molecular and cluster systems. Additionally, the group has expertise in 1D/2D/3D periodic models and performs a wide range of density functional theory calculations in conjunction with these models (Castep, ADF, Quantum-Espresso, CPMD, CP2K, VASP) for describing the heterogeneous interactions taking place on surfaces or in the bulk of materials, and for analyzing the mechanical, thermochemical, electronic, optic, and magnetic properties of gas, liquid, and solid systems of interest.

Classical mechanics-based simulation capabilities. The team uses both academic or commercial packages (e.g., DL-POLY, Charm, Gromacs, Amber, NAMD, LAMMPS, and Discover), as well as in-house developed software packages, to characterize the dynamic properties of molecular systems in different statistical ensembles. These software packages allow the team to obtain the essential metrics responsible for gas separation and capture processes, or to determine parameters that can be correlated directly to experiments such as adsorption isotherms and selectivity or solubility of different gases adsorbed in nanoporous or heterogeneous solid-liquid materials. Several of these simulations include in-house, first principles-based molecular force fields.

Mesoscale-based simulation capabilities. The team's computational capabilities in kinetic Monte Carlo and microkinetic modeling areas use the thermochemical information obtained at quantum mechanics level to determine information essential to correlating atomic-scale behavior with experimental measurements, such as reaction rates or concentration profiles at different temperature and pressure conditions. Such information is vital for accurate large-scale computational fluid dynamics simulations or reactor design.

Multiscale computational capabilities. The team aims to correlate nanoscale and macroscale properties to describe phase diagrams and microstructure evolution of alloys. This will create a better understanding of materials performance for service life duration, to optimize heat treatment processes by taking advantage of existing thermodynamic and kinetic databases, or to evaluate the electromagnetic field evolution in complex media.

ON-SITE FACILITIES

High-performance computational facilities. The CME Team's expertise has grown in direct correlation with the development of large-scale, highly parallel supercomputer systems. For this reason, NETL has acquired and continues to develop some of the largest and most efficient supercomputer capabilities in the country. The supercomputer systems at NETL, in conjunction with CME Team's technical capabilities, allow the use of highly complex and demanding computational models, which can provide highly accurate physical-chemical properties, accelerate discovery overall, and provide better guidance to the experimental development of novel materials with optimized properties.

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ON-SITE RESEARCH

Computationally optimized heat treatment of metal alloys. Conventional processes for homogenizing metal alloys are trial and error in their approach, resulting in increased process cost and limits to the possible paths that may be explored. NETL's computationally optimized homogenization heat treatment process provides an easy method to optimize heat treatment to achieve the desired degree of homogenization with minimum furnace time.

The primary application for this technology is for alloys that are exposed to extreme environments, including heat-resistant alloys or those needing corrosion/oxidation resistance. A properly homogenized alloy will not only perform better but will also have an extended life cycle.

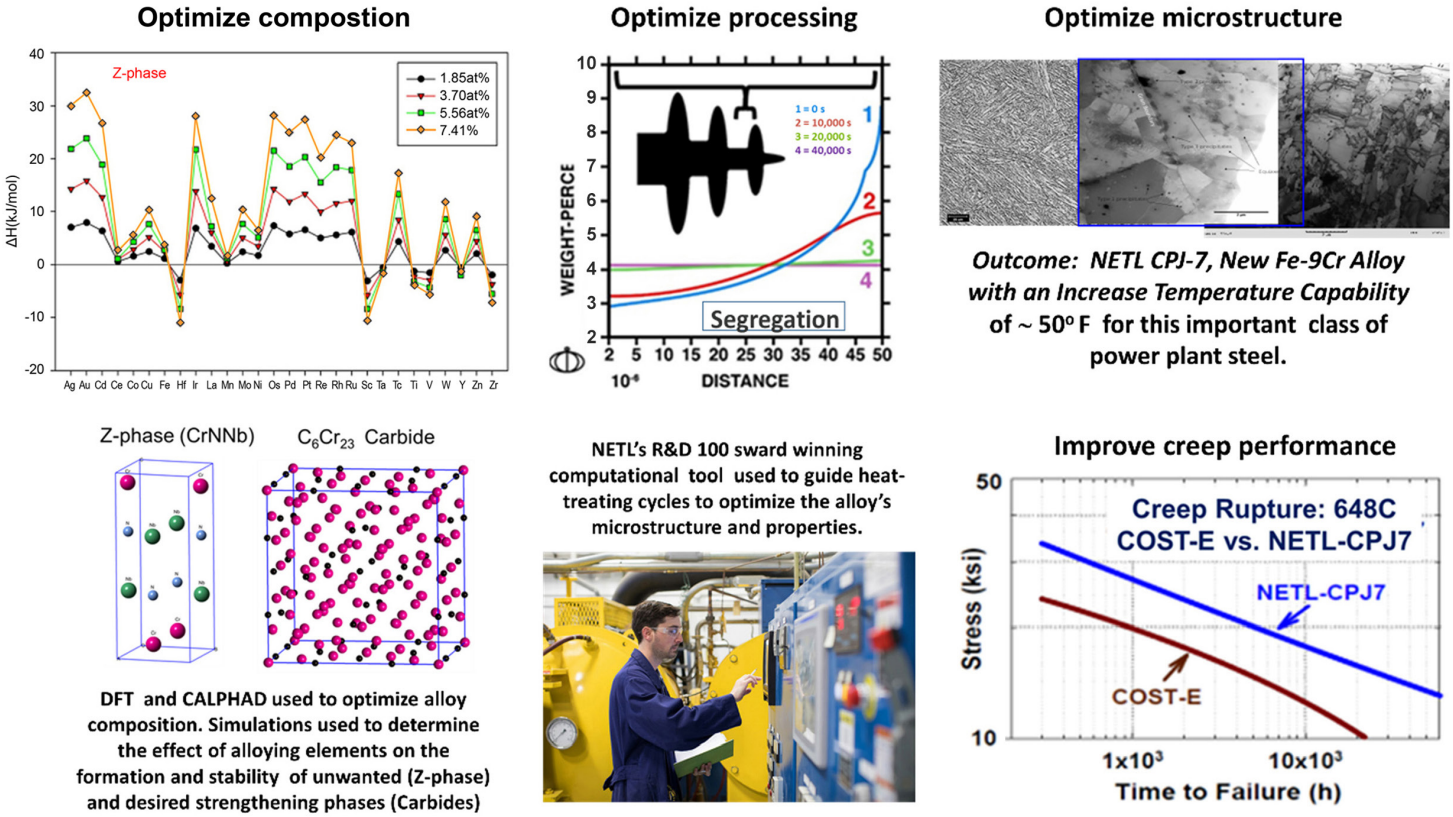

Figure 1. The alloy development process can be optimized though computational science.

Computational visualization for Carbon Dioxide to Carbon Monoxide conversion. NETL has shown gold (Au) nanoclusters are extremely efficient catalysts for converting carbon dioxide (CO_2) into carbon monoxide (CO). Copper-gold (Cu-Au) nanoalloys were developed to selectively convert CO_2 into CO with reduced precious metal content. The Au-Cu nanocluster structures were generated by Materials Studio, an atomic structure visualization software. The Vienna Ab Initio Simulation Package (VASP) was then used to generate structural, electronic, and vibrational information. By using an in-house computational electrochemistry code, catalytic reactions were simulated on Au-Cu nanoclusters under electrochemistry conditions. Density functional theory calculations were performed on NETL's Joule supercomputer. The alloys retained the activity and selectivity of pure gold with an approximately 50 percent reduction in precious metal content. This development paves the way for less expensive CO_2 utilization catalysts that can convert CO_2 and water into synthesis gas (CO + H_2).

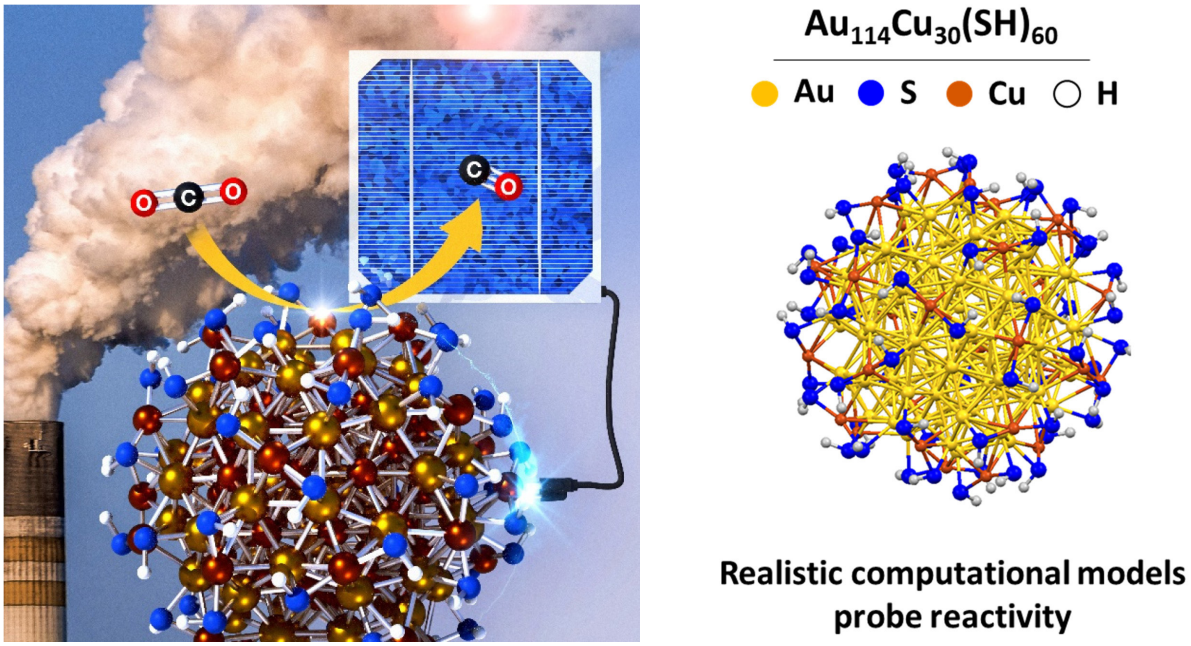

Figure 2. Au-Cu nanocluster structures.

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