Richard P. Feynman Center for Innovation

Technology Snapshot

Technology Licensing Opportunity

Los Alamos NATIONAL LABORATORY

Architector 2.0

Automated 3D structure generation and evaluation for metal–ligand complexes

Value Proposition

Architector 2.0 is advanced scientific software that helps researchers design and evaluate new metal-based compounds essential for technologies that support clean energy, electric vehicles, advanced manufacturing, nuclear fuel recycling and certain medical treatments. By allowing scientists to rapidly test thousands of possible chemical combinations virtually before making them in the lab, Architector significantly reduces the time, cost and uncertainty involved in discovering new materials.

Technology Readiness Level 6

Contact Information

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Please reference C22085 when reaching out.

Overview

Architector 2.0 automatically builds and evaluates chemically realistic three-dimensional models of metal–ligand complexes across the periodic table from minimal chemical input. By generating multiple plausible structures and ranking them using physics-based and data-driven methods, the software enables rapid exploration of complex inorganic chemical space, including difficult rare earth and actinide systems. This capability reduces the time, cost and uncertainty of molecular design and supports discovery in catalysis, nuclear fuel cycle science, energy technologies and advanced materials.

Advantages

- **Accelerates discovery across the periodic table** – Automates exploration of diverse metal–ligand systems, including difficult f-block elements, through high-throughput workflows and advanced 3D functionalization.
- **Improves chemical predictivity** – Models secondary solvation shell effects, including solvent and counterions, to produce more realistic and reliable structural predictions.
- **Expands access with an intuitive GUI** – Provides a user-friendly interface that enables both experts and non-experts to explore complex chemical spaces efficiently.
- **Reduces cost and experimental risk** – Combines efficient ligand sampling with machine learning–guided conformational exploration to minimize trial-and-error and accelerate decision-making.

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NNSA National Nuclear Security Administration

Technology Description

Architector 2.0 is a computational software platform designed to automatically generate chemically realistic three-dimensional models of metal–ligand complexes across the periodic table. The software begins from minimal chemical inputs, such as a description of the metal center, ligand structures and key electronic properties, and then constructs a diverse set of plausible molecular geometries that satisfy known chemical and structural constraints. These candidate structures are evaluated using a combination of physics-based models and data-driven approaches to identify energetically reasonable configurations. By systematically generating and ranking multiple conformations, Architector enables researchers to capture the structural diversity that often governs the behavior of metal complexes in real chemical environments. This automated approach replaces what has traditionally been a manual and time-intensive process in computational chemistry.

The platform is designed to operate at high throughput and can scale from individual desktop systems to high-performance computing environments, allowing researchers to evaluate thousands of candidate compounds in parallel. This capability makes it possible to explore large regions of chemical space and rapidly identify promising compounds for further theoretical study or laboratory synthesis. Architector can also generate chemically meaningful environments surrounding a complex, enabling more complete evaluation of molecular stability and interactions. By providing reliable initial structures and configuration searches for challenging metal systems—including rare earth and actinide complexes—the software supports computational workflows used in catalysis research, nuclear chemistry, advanced materials development and molecular design for energy and environmental applications.

Market Applications

- **Critical Materials & Mining** (rare earth element separation, strategic mineral processing)
- **Nuclear Energy & Fuel Cycle** (fuel recycling, radioactive waste reduction, advanced reactor materials)
- **Energy & Clean Technology** (energy storage materials, catalysts for clean fuels, carbon management technologies)
- **Chemical Manufacturing** (industrial catalysts, specialty chemicals, process optimization)
- **Pharmaceuticals & Medical Isotopes** (metal-based therapeutics, diagnostic imaging agents)
- **Advanced Materials & Electronics** (magnetic materials, functional coatings, next-generation electronic materials)

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