



ChemOS

A portable, modular, and versatile open-source orchestration software for operating autonomous/self-driving chemistry and materials science laboratories.

<https://github.com/aspuru-guzik-group/ChemOS>

Overview

ChemOS is a software package developed by the Aspuru-Guzik Group at the University of Toronto designed to supply the structured layers indispensable for the deployment and operation of autonomous or "self-driving" laboratories (SDLs).

Its primary goal is to democratize and accelerate scientific discovery in chemistry and material science by bridging the gap between automated robotic platforms, artificial intelligence, and high-performance computing. The software enables a closed-loop approach to experimentation, where experiments are iteratively designed on-the-fly by a machine-driven decision-maker based on previously conducted experiments.

ChemOS follows a modular architecture composed of a central workflow manager and six independent modules:

AI Algorithms for Experiment Planning (Learning Module): Incorporates state-of-the-art machine learning methods, such as Bayesian optimization algorithms like Phoenix and SMAC, to suggest optimal experimental conditions.

Automation and Robotics: Manages the execution of experiments on automated robotic platforms.

Characterization Equipment: Integrates with equipment to assess the performance of conducted experiments and provide feedback.

Databases Handling and Management: Coordinates data collection and long-term data storage, supporting systems like SQLite.

Intuitive Interfaces for Researchers: Facilitates interaction with researchers, including an NLP module in a chatbot framework for remote command and instruction.

Online Results Analysis: Features an analysis module for pre-processing, summarizing, and visualizing experimental results, including time traces and search space visualization.

This modularity decouples interdependent tasks, allowing for easy extension and simplified deployment to new applications by only modifying a configuration file. It also supports remote control of laboratories and access to distributed computing resources.

Key Features

- Autonomous Experiment Planning (AI/ML)
- Robotics and Automation Control
- Modular Workflow Manager
- Real-time Data Acquisition and Analysis
- Remote Laboratory Control
- Intuitive Researcher Interface (Chatbot/NLP)
- Database Management

Pricing

Model: free

ChemOS is an open-source software package available for free on GitHub, developed by the Aspuru-Guzik Group at the University of Toronto.

Target Company Size: startup, small, medium, enterprise

Integrations

Phoenics (Bayesian Optimizer), SMAC (Algorithm Configuration), SQLite, Automated Robotics Equipment (via APIs), Characterization Equipment (via APIs)

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