

Jaqpot: A computational cloud platform supporting the design of safe and sustainable chemicals and materials

Alex Arvanitidis¹, Vasileios Minadakis¹, Giannis Savvas¹, Periklis Tsiros¹, Philip Doganis¹, Haralambos Sarimveis¹

¹ School of Chemical Engineering, National Technical University of Athens, Attiki 15772, Greece, hsarimv@central.ntua.gr, http://chemeng.ntua.gr/labs/control_lab/

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Abstract

The successful introduction of innovative advanced materials and chemicals (AMCs) in a safe-and-Sustainable-by-Design (SSbD) Framework requires achieving an optimal balance of safety, sustainability, functionality and cost-efficiency [1,2]. Computational approaches aim at implement the “by-Design” approach by formulating and solving optimization problems that identify combinations of properties across these four categories, thereby enabling targeted materials innovation. This challenge is addressed by Jaqpot, an open-source platform designed to facilitate the development, deployment, and management of machine learning (ML) models and other computational models, such as Physiologically Based Kinetic (PBK) models, specifically tailored for chemicals and materials modelling applications (<https://app.jaqpot.org/>).

Jaqpot’s user-friendly interface and robust APIs allow users to upload, manage, and deploy custom models while also accessing a repository of pre-existing models. Users do not need to own, set up, or maintain heavy computational infrastructure, as the computational costs are covered by cloud infrastructure, with the option for private installations. Additionally, users of the platform have the ability to create private organisations accessible only to invited users, each with their specific privileges. The platform incorporates advanced preprocessing and featurization techniques, enhancing model accuracy and interpretability. Key features include cloud-based deployment, ensuring access to the latest libraries and technologies, and compatibility with popular ML frameworks such as Torch, Scikit-Learn, and ONNX runtime. Furthermore, the Python client, Jaqpotpy, streamlines interactions with the platform, enabling automated workflows for efficient model management. Jaqpot is being expanded to include generative learning approaches and Large Language Models (LLMs), further supporting the SSbD concepts. Detailed documentation is provided at <https://jaqpot.org>.

By addressing common challenges in the ML lifecycle—such as data security, collaboration, and model performance—Jaqpot empowers materials scientists to focus on innovation rather than infrastructure.

References

[1] European Commission: Joint Research Centre, Caldeira, C., Farcas, R., Moretti, C., Mancini, L. et al., Safe and sustainable by design chemicals and materials – Review of safety and sustainability dimensions, aspects, methods, indicators, and tools, Publications Office of the European Union, 2022, <https://data.europa.eu/doi/10.2760/879069>

[2] European Commission: Joint Research Centre, Abbate, E., Garmendia Aguirre, I., Bracalente, G., Mancini, L. et al., Safe and sustainable by design chemicals and materials – Methodological guidance, Publications Office of the European Union, 2024.

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