Engineering biology solutions to advance cultivated meat engineering

Dr Francesca Ceroni

The Ceroni lab, embedded in the dept of Chemical engineering, the Bezos centre for sustainable protein, the national alternative protein innovation centre and the EEBio programme grant at Imperial College London, is seeking outstanding candidates interested in applying engineering biology to mammalian cell engineering for host-aware bio controller designs and for cultivated meat applications.

Learning-based Strategies in Deterministic Global Optimisation of MINLP Models in Chemical Engineering

Professor Benoit Chachuat

This PhD project will focus on advancing deterministic global optimisation methods for mixed-integer nonlinear programming (MINLP) models in chemical engineering by integrating machine learning and reinforcement learning techniques. Deterministic global optimisation provides rigorous guarantees for handling the nonconvexities and combinatorial complexity inherent in MINLP formulations of process design, synthesis, and scheduling problems, but it often suffers from prohibitive computational cost. The project will explore how data-driven surrogates and learning-based strategies can accelerate key algorithmic components, such as bound tightening, branching decisions, cut generation, and the combination of effective relaxation techniques. In particular, reinforcement learning will be investigated to guide search strategies adaptively, improving efficiency in exploring the solution space while maintaining global optimality guarantees. By combining the reliability of deterministic optimisation with the adaptability of modern learning methods, this research aims to deliver scalable and agile optimisation tools and software that unlock new possibilities for computer-aided molecular and process design, enterprise-wide process optimisation, and sustainable process systems engineering.

Data-driven process control via reinforcement learning and large language models

Dr Antonio del Rio Chanona

You will develop data-driven methodologies for to control chemical processes by combining reinforcement learning (RL) with large language models (LLM). The aim is to be able to control complex and uncertain processes using RL to learn effective decision-making policies, while leveraging LLMs to integrate prior knowledge, guide exploration, and as a supervisory agent. You will develop and learn programming skills (Python) as well as machine learning and artificial intelligence theory and practice.

Developing self-optimising processes via Bayesian optimisation and machine learning

Dr Antonio del Rio Chanona

You will develop methodologies to design and operate self-optimising chemical processes by combining Bayesian optimisation (BO) with machine learning (ML). The aim is to efficiently explore and improve process conditions under uncertainty, using BO to guide experiments and simulations towards optimal performance, while applying ML models to capture complex system behaviour and enable faster decision-making. You will develop and strengthen programming skills (Python) as well as gain theoretical and practical knowledge in optimisation, data science, and machine learning for process systems engineering.

Addressing key challenges in energy systems modelling for the 21st century

Professor Adam Hawkes

Possible projects focus on treatment of uncertainty, modelling fit of high VRE high storage systems, rapid energy model creation using LLM and ML techniques, and integrating sustainable and equitable development principles in modelling frameworks.

Statistical mechanical modelling of the themophysical properties of complex fluids and materials

Professor George Jackson

A molecular description of matter is the key to understanding and predicting the properties of dense fluids and materials. The latest developments in statistical mechanical theories and computer simulation (Monte Carlo and molecular dynamics) are used in the Molecular Systems Engineering (MSE) group to provide a reliable predictive platform for complex fluids and ordered materials at the molecular level. The focus is on the phase equilibria of systems which are of industrial relevance, e. g., mixtures containing hydrogen fluoride (production of refrigerants), amines (processes for carbon capture), aqueous solutions of surfactants (enhanced oil recovery, structured phases), liquid crystals (optical devices), and active pharmaceutical ingredients (drug formulation and processing).

Novel optical measurments for developing clean energy solution

Professor Christos N. Markides

In this project we will use novel laser-based techniques to characterise fluid processes that are critical for the future of clean energy technologies. We will investigate special fluids that open new possibilities for clean cooling and energy conversion, including supercritical fluids. This is a blend of theoretical work and experimental work, while contributing to clean energy transition.

Next generation multi-functional PV-X technologies for multigeneration from the sun

Professor Christos N. Markides

This project involves combined computational modelling, design and experiments on advanced PV-X collector architectures. A coupled optical, electrical, thermal and electrochemical model will be developed to design the collector, followed by fabrication and testing to confirm performance.

Cutting-edge synergetic compressed-air and hydrogen grid-scale electricity storage solutions

Professor Christos N. Markides

Through advanced in silico designs of a new energy storage technology, is project aims at optimising its performance, and exploring its value and wider role within the energy system. By recovering and valorising the heat generated during charging of a compressed air electricity storage plant to drive high-efficiency high-temperature water electrolysis, the proposed innovative system allows emission-free and cost-effective inter-seasonal (and beyond) electricity storage, key for a sustainable energy future.

Application of CFD, Machine Learning, and Shape Optimization to flow chemistry applications

Professor Omar Matar

Mixing reactors are used in chemical synthesis, polymerisation or pharmaceutical manufacturing. Computational fluid dynamics (CFD) simulations for these reactors are expensive, and solutions obtained are specific to the particular flow and geometry condition, making the evaluations based on various geometries for design improvements challenging. To overcome this challenge, we will aim to build faster machine-learning based surrogate models with the focus is on handling high-dimensional simulation data for complex reactor geometrical parameters. The proposed model will leverage advanced deep learning techniques, specifically graph neural networks (GNNs) and specialised convolutional neural network (CNN) autoencoders. GNNs are chosen for their ability to capture geometric and topological information effectively, making them suitable for representing complex geometrical features in fluid dynamics. On the other hand, CNN autoencoders are expected to learn a compressed representation of fluid dynamics, facilitating efficient simulation of high-dimensional data. This approach aims to significantly improve computational efficiency and accuracy in fluid dynamics simulations, especially in scenarios with varying flow rates, and geometric configurations. The project's success will be measured by the surrogate model's ability to outperform traditional CFD methods in terms of computational efficiency and accuracy, as well as its robustness and flexibility in handling different fluid flow scenarios.

Modelling, simulation, and optimization of impinging jet mixers for pharma applications

Professor Omar Matar

This project applies modelling and simulation to investigate impinging-jet mixers, a key technology in pharmaceutical manufacturing where precise mixing governs product quality and consistency. Computational fluid dynamics (CFD) models are developed to capture the complex hydrodynamics, turbulence, and mass transfer phenomena occurring when two or more liquid jets collide at high velocity. Simulation results provide insight into mixing efficiency, energy dissipation, and micromixing timescales critical for crystallization, nanoparticle synthesis, and formulation processes. By linking model predictions with process performance, the study supports optimization of mixer design and operating conditions, reducing experimental effort while enhancing scalability and regulatory robustness.

Human centric AI solutions for assisting chemical process control operators

Dr Mehmet Mercangoz

Designs AI copilots that augment, not replace, control-room operators. Combines physics-guided analytics with interpretable ML to surface early warnings, suggest constraint-safe actions, and explain rationales in plain language. Emphasis on trust, usability, and closed-loop performance under anomalies and long-tail events.

Application of AI for supporting industrial decarbonisation: handling operational complexity with intelligent systems

Dr Mehmet Mercangoz

Applies intelligent systems to cut emissions while preserving throughput and quality across complex, multi-unit sites. Uses hybrid digital twins, online optimisation, and decision support to coordinate energy use, schedule low-carbon modes, and exploit flexibility (fuel switching, demand response, heat integration). Delivers measurable CO_2 reduction with auditable, operations-grade recommendations.

Control and optimization of high temperature heat pumps

Dr Mehmet Mercangoz

Develops advanced control, estimation, and supervisory optimisation for industrial HT-HPs delivering 120–500 °C process heat. Integrates with industrial waste-heat sources (variable temperature/flow, intermittent availability) via hybrid digital twins that characterise source quality in real time and route heat through recovery networks. Uses model-predictive control, health-aware set-points, and grid-responsive operation to maximise COP, stabilise transients, and cut life-cycle cost while electrifying process heat at scale.

Design of sustainable fluids using machine learning and molecular simulation

Professor Erich Muller

We are seeking highly motivated candidates for fully funded PhD projects at the exciting interface of molecular simulation and machine learning to design the next generation of sustainable fluids. This pioneering research focuses on creating environmentally benign lubricants, solvents, and refrigerants from the ground up by computationally predicting their physical, chemical, and environmental properties. In this project, you will employ state-of-the-art molecular dynamics and Monte Carlo simulations to generate vast datasets of molecular behaviour, which you will then use to train sophisticated machine learning models. The ultimate goal is to develop an innovative in silico framework that rapidly screens and optimises novel chemical structures, accelerating the discovery of high-performance, non-toxic, and biodegradable fluids to solve critical industrial and environmental challenges. Ideal applicants will have a strong background in chemistry, physics, chemical engineering, or a related discipline, with a keen interest in computational science and a passion for sustainability.

Machine-learning enhanced Mixed Integer optimisation for circular, biopharma symbiosis

Dr Maria Papathanasiou

The Papathanasiou lab is seeking for motivated PhD candidates who are passionate about digital tool development and their application in biopharma. The (bio-)pharmaceutical industry is challenged to ramp up its global capacity, while working to meet net-zero targets, ensuring continuous drug supply. Beyond the geopolitical challenges faced worldwide, (bio-)pharmaceutical processes have been historically very complex to design, optimise and integrate in a global distribution network that is resilient and adaptable to change. In that, digital tools, assisted by Artificial Intelligence, can revolutionise the state-of-the-art in biopharma manufacturing and supply chains, offering a cost-effective solution to improve performance and increase resilience. This research area investigates how a portfolio of digital solutions, can identify and quantify manufacturing uncertainties and estimate their impact on drug supply. Projects are focused both on digital design space identification for improved manufacturing regimes that meet, as well as supply chain optimisation focusing on the integration of economic, social and environmental sustainability.

Integrated design and control for sustainable biopharma manufacturing via Reinforcement Learning

Dr Maria Papathanasiou

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AI for Antibody and Protein Design

Dr Pietro Sormanni

Help build the next generation of AI tools for designing therapeutic antibodies and proteins. The project develops and evaluates machine-learning methods to generate sequences with improved specificity, stability, solubility and reduced immunogenicity. Approaches may include repertoire-scale foundation models, geometrical deep learning, diffusion models, and multi-objective optimisation, linked to experimental feedback from our protein-biophysics assays. Outcomes will be open, usable tools applied to real design problems with implication for fundamental and applied research, also in partnership with industry. There is scope to refine the methodological focus to your interests (e.g., generative models, active learning, interpretable AI, sequence–structure integration). Applicants should enjoy coding (Python) and quantitative thinking; prior ML experience is welcome but not essential if motivation is high.

Engineering single-domain antibodies: from selection to drug-like leads

Dr Pietro Sormanni

Discover and improve nanobodies – single-domain “mini-antibodies” with major potential for therapeutics and diagnostics. You will use in-vitro display selections (ribosome or yeast display) to isolate binders to medically relevant targets, then analyse and refine post-selection libraries to understand and predict how sequence affects binding and developability. Laboratory work (molecular biology, expression/purification) is paired with data analysis and computational method development to guide candidate selection and iterative optimisation. The goal is to deliver robust leads with real-world impact in health and biotechnology. There is genuine scope to shape targets and techniques to your interests. Applicants from biochemistry, molecular biology, chemical engineering or related fields are encouraged to apply.