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IMPERIAL Grantham Institute

**Project title:** Design of smart, multifunctional photonic systems for solar-driven carbon capture and conversion

**Lead Supervisor and Department:** Xiangkun (Elvis) Cao, Department of Mechanical Engineering

**Project Description:**

One of the key barriers to the photo-driven processes is the inherent low efficiency. By introducing other energy sources, such as thermal, electric, magnetic, ultrasonic, microwave, or mechanical energy into photo-driven systems, we could achieve efficient synergetic effects and drive chemical systems (e.g., catalytic reactions) more efficiently and sustainably. Taking photothermal systems as an example, the design of such hybrid systems poses a multiscale challenge. At the microscale, there is a gap in the concurrent transport and delivery of photons, phonons, and molecules to reaction sites with microscopic precision. At the cell scale, we need to co-design optical, thermal, and mechanical components tailored to the energy carriers (i.e., photo- and thermal-) involved in the process. At the process scale, incorporating multiple energy sources poses a concurrent optimisation challenge for the various design and operating parameters of such systems.

The PhD project will focus on tackling such multiscale design challenges tailored for photothermal-driven reactions. The target application is solar-driven carbon management (e.g., carbon capture, carbon conversion, integrated carbon capture and conversion). Traditional carbon management systems powered solely by photochemistry usually have low efficiencies, whereas processes powered solely by thermal chemistry incur a high activation energy barrier. By integrating photo- and thermal processes, we could fully utilise the solar spectrum and enhance chemical conversion efficiencies under mild conditions. Photochemistry has the effect of reducing the activation energy barrier, while temperature enhances the probability of reactants overcoming the barrier by providing additional thermal energy.

The PhD project will involve investigations at three scales. At the microscale, this involves developing a microscopic understanding of the concurrent transport and conversion of photons, phonons, and molecules, leveraging physics-informed ML to enhance numerical approaches. The student is expected to design pathways to maximise solar irradiation capture and minimise parasitic absorption, reflection, scattering, transmission, and thermal conductive, convective, and radiative losses. This also involves building theoretical models of photon and phonon transport and conversion, and embedding these models in simulations such as Monte Carlo methods. There is also potential to embed physics-informed ML into the design and optimisation of the transport and conversion of photons and phonons.

At the cell scale, this involves co-designing optical, thermal, and mechanical components tailored for various solar-driven carbon management technologies, leveraging advanced manufacturing tools (e.g., 3D printing) for rapid prototyping and experimental testing. Multiphysics modelling informs the understanding of the effect of different design and operating parameters on reactor performance. Advanced manufacturing of components can reduce capital and operating costs, speed up construction, and increase reliability. The proposed work builds on the group’s deep experience in designing and optimising multi-component, multi-phase reactors, manufacturing devices with ideal geometries and surface structures, and conducting optimisation to enhance reactor performance.

At the process scale, this involves designing and optimising pathways to maximise system co-benefits and minimise risks during operation, leveraging ML for process design and optimisation. There are vast opportunities to achieve system co-benefits (e.g., enhanced energy efficiency) and minimise risks (e.g., environmental impacts) by integrating solar-driven carbon management systems with existing infrastructure. For example, the group's recent work integrating direct air capture (DAC) units with building HVAC systems to achieve concurrent carbon removal and improved energy efficiency is compelling.

The student will engage in the associated PhD training and activities of the Grantham Institute – Climate Change and Environment and the Department of Mechanical Engineering.

**How to apply:**

Please email Xiangkun (Elvis) Cao and include in your application:

- Statement of Purpose
- Your CV
- At least two references to be sent directly to Xiangkun (Elvis) Cao from the referees.

Informal enquiries are welcomed and should be sent to Xiangkun (Elvis) Cao