Predicting Nanozyme Activity: How Protein Coronas Reshape Catalysis
EPSRC funded PhD studentship with full fee waiver and £21,805 pa stipend (2026/27 rate)

Project Code: DLA_DTP_2026_05

Main Supervisor: Dr Marco Molinari

Co-Supervisor: Dr Joanna Fox, Dr Stavros Christopoulos

Project Introduction

When nanoparticles enter biological environments, their high surface energy triggers the spontaneous adsorption of proteins, forming a protein corona. In healthcare technology, this shell redefines the nanoparticle's "biological identity," often masking engineered targeting ligands and leading to rapid immune clearance.

For nanozymes, the impact is significant as the protein layer physically blocks active catalytic sites, severely diminishing their therapeutic efficiency. Consequently, while the corona can be engineered for controlled drug release, it generally complicates clinical translation by reducing predictability and precision. Managing this interface is essential for developing reliable, high-performance nanozymes for diagnostics and targeted therapy.
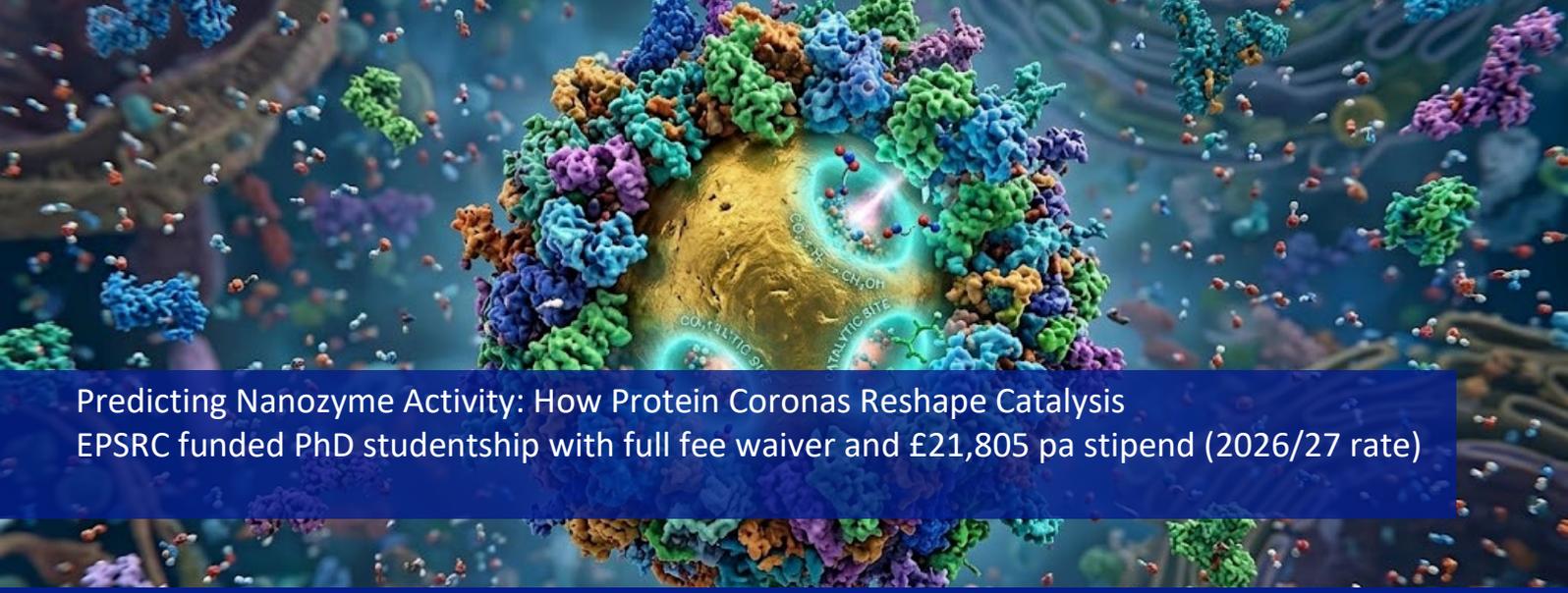
Project Details

Nanozymes are nanomaterials with intrinsic enzyme-like activities and offer superior stability and cost-effectiveness compared to natural enzymes. However, their performance in biological environments is dictated by the protein corona, a spontaneous coating of proteins that can physically block active sites or chemically alter the nanozyme surface electronic structure. This proposal aims to simulate these complex interfaces to predict how the protein corona modulates nanozymatic activity. This research will provide a predictive framework for designing responsive nanozymes that maintain high activity even in protein-rich environments.

Understanding this interface requires a multiscale computational approach, as the system is too large for pure quantum mechanics but too chemically complex for standard force fields.

1. Stage 1: Benchmarking will utilize Density Functional Theory (DFT) to characterize the interaction of the building-block amino acids onto candidate nanozyme surfaces. These simulations will provide high-accuracy data on binding energies, charge transfer, and adsorption geometries.

2. Stage 2: Machine Learning Interatomic Potentials (MLIP) will be retrained using the DFT dataset. These will achieve near-DFT accuracy at a fraction of the computational cost, enabling the simulation of the complex interactions between the nanozymes and the proteins

3. Stage 3: The evaluation of the catalytic activity of nanozymes surfaces will be investigated taking into consideration the orientation and deformation of proteins on the nanozyme surface correlate with a reduction or enhancement in catalytic turnover.

This proposal marks a shift from trial-and-error discovery to the rational design of nanomedicine. By decoding the "biological identity" imposed by the protein corona, this research transforms nanozymes from lab curiosities into robust healthcare tools. Utilizing a multiscale computational framework will predict and prevent the "poisoning" of catalytic active sites. This will enable the creation of stable, more durable, diagnostic sensors that maintain efficacy in protein-rich environments. Ultimately, this work will bridge the gap between materials science and physiology, paving the way for predictable, high-performance nanotherapeutics that function reliably within the complex chemistry of life.

Project-specific entry requirements

Applicants should have, or expect to achieve, at least a 2.1 honours degree, in Chemistry, Physics, Materials Science, and other relevant STEM degrees. Previous knowledge on simulation methods or programming is desirable but not necessary.

Further Information

This call is open to **UK Applicants only**.

Applicants should be of outstanding quality and exceptionally motivated.

The studentships are funded for 3 years (subject to satisfactory annual performance and progression review) and will provide for tuition fees and a tax-free stipend paid monthly.

Please note that there are more projects than funded studentships available and therefore this is a competitive application process which will include an interview. Shortlisted candidates will be contacted for an interview in person or via Teams. After interview the most outstanding applicants will be offered a studentship.

Queries about the application process are welcome and should be emailed to pgrscholarships@hud.ac.uk.

Informal enquiries about this project should be directed to Dr Marco Molinari.

Type of Award: Doctor of Philosophy (PhD).

Eligibility: UK applicants only. First Class or Upper Second-Class Honours degree or equivalent in a relevant subject area, please refer to the entry requirements on the specific projects being advertised.

Location: Huddersfield.

Funding: 3 years full time research covering tuition fees and a tax-free bursary (stipend) starting at £21,805 for 2026/27 and increasing in line with the EPSRC guidelines for the subsequent years. Funded via the Engineering and Physical Sciences Research Council Doctoral Training Programme.

Duration: 3 years full-time plus 12 months writing up (please note that no funding is available for the writing up period).

Closing date: 28th April 2026

Start date: 1st October 2026

Application details

- Go to the EPSRC webpage and download the Expression of Interest Form 2026.
- Provide copies of transcripts and certificates of all relevant academic and/or any professional qualifications.
- Provide references from two individuals – please contact your referees and ask them to send them directly to pgrscholarships@hud.ac.uk from their email address.
- Proof of eligibility – e.g. scan of passport photo page
- Completed forms, including all relevant documents should be submitted via-email to pgrscholarships@hud.ac.uk.

Please note: if you do not attach all the relevant documentation prior to the closing date your application will not be considered.