Wenyi FENG

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Computational chemist experienced in molecular dynamics simulations techniques and Python programming;

Passionate about exploring state-of-art computational chemistry techniques.

Education

PhD Pharmacy **University College London** **October 2021 - January 2026**

MS Drug Design (Distinction) **University College London** **September 2020-September 2021**

Core modules: Bioinformatics and structural biology as applied to drug design, Cheminformatics and modelling for drug design, Fragment based drug design and virtual screening.

BS Applied Chemistry (overall score: 85.7%) **Huaqiao University** **September 2016-July 2020**

Experience

Lab experience

- **PhD thesis 'Evaluation of the GCPQ as drug delivery system using atomistic molecular dynamics simulation and experimental methods'**
  - Independently established atomistic molecular dynamics (MD) simulation workflows for chitosan-based amphiphilic polymers as the sole computational chemist in the group.
  - Designed and executed MD simulations to predict physicochemical properties of single-chain, self-assembled, and drug-loaded polymer systems.
  - Elucidated molecular mechanisms of polymer self-assembly and drug encapsulation, providing insights to guide rational formulation design.
  - Developed custom Python scripts for MD trajectory analysis, data processing, and structural visualisation.
  - Collaborated in Design of Experiments (DoE) to support experimental planning, execution, and optimisation of polymer synthesis protocols.
  - Contributed to proteomics data analysis from LC–MS using R in collaboration with senior researchers.
  - Performed polymer characterisation using NMR, DLS, GPC–MALLS, and HPLC to validate computational predictions.
- **Master thesis 'Effects of QPR and Environmental Factors on GCPQ Nanoparticle Formulation and Colloidal Stability'**
  - Investigated the effects of formulation conditions (pH, salt concentration, formulation techniques) on the physicochemical properties of chitosan-based amphiphilic polymers.

Working experience

- Postgraduate teaching assistant for UPCSE chemistry in UCL IOE September 2023-July 2025

Mentored groups of pre-undergraduate students on lab practices including titration, organic synthesis, analytical techniques etc.

Conference and presentation experience

- Presented poster, 'Mechanism of curcumin encapsulation by GCPQ polymers: unexpected polymer mesh (matrix) configuration revealed by atomistic molecular dynamics simulations', at AAPS PharmSci360, Salt Lake City, USA, October 2024
- Presented poster, 'All-atom MD simulation of modified chitosan polymer GCPQ suggest self-assembly into a nano-sized gel matrix', and presented lecture, 'Molecular dynamics simulation and experimental methods to understand GCPQ as drug delivery systems', on UCL School of Pharmacy Research Day, September 2024
- Presented poster, 'Atomistic MD simulation of modified chitosan polymer GCPQ suggest self-assembly into a nano-sized gel matrix', on RSC Molecular Simulations in Chemistry conference, London, UK, June 2024

- Presented poster, 'Atomistic molecular dynamics simulations of modified chitosan polymer GCPQ suggest self-assembly into a nano-sized gel matrix', on TYC student day, London, UK, May 2024
- Presented poster, 'Experimental and molecular modelling methods to understand GCPQ as drug delivery system', on TYC student day, London, UK, May 2023

Leadership experience

- Director of Organizational Department of the 19th League Committee, Huaqiao University June 2017- June2018

Collaborated with teachers and peers to host discussion forum to bridge communications as main member of League committee (the Student Union); Organized various extracurricular activities for peers (highly recognized by participants).

Skills

Molecular Modelling & Simulation:

- Polymer model construction using Tcl scripting (PSFGEN) and semi-quantum mechanical calculations for HOMO–LUMO analysis and reactive site identification
- Atomistic molecular dynamics simulations using Schrödinger Maestro/Desmond, including system setup, execution, and validation
- MD trajectory visualisation and structural analysis using VMD
- Polymer–drug interaction analysis using the Schrödinger Python API

Data Analysis & Programming:

- Data processing, statistical analysis, and visualisation using Python (Jupyter) and R
- Workstation and cloud desktop management in Linux (Ubuntu) environments, including job submission, file system organisation, and software environment configuration

Drug Design:

- Molecular docking using GOLD
- Structure-based virtual screening and homology modelling using MOE
- Cheminformatics and molecular manipulation using RDKit

Experiments: organic synthesis, polymer synthesis, nanoparticle characterisation, drug formulation, DLS, HPLC, NMR, GPC-MALLS, TEM, XRD, Rheometer

Awards

- Best lecture (people's choice) prize on UCL SoP Research Day, September 2024
- Best poster prize (1 of 3) on Thomas Young Centre Student Day, out of 45 posters, May 2023
- First-class Scholarship of Huaqiao University, for ranking 2nd in overall score containing exam marks and extracurricular performances, out of 50 students in class, December 2019