An IPR seminar series supported by
WPI-PRIMe and ASPiRE

BioSim Talk #5

Joshua Lam

University of Manchester,
Manchester Institute of Biotechnology & Department of Chemical Engineering, UK
Bioinformatics Institute, A*STAR, Singapore

26th August 2025 (Tuesday)
4.00 – 5.30 pm
Institute for Protein Research
University of Osaka (Suita Campus)
4th floor seminar room

The Polarisation Effect: Small Tweaks, Big Effects in Classic Molecular Simulations

Molecular dynamics (MD) simulations provide detailed insights into the atomistic mechanisms of complex biological processes, many of which remain difficult to access experimentally. However, the reliability of these simulations hinges on the accuracy of the employed force fields. A well-known limitation of classical force fields is their tendency to overestimate electrostatic interactions, particularly in systems involving polyvalent ions, due to the neglect of electronic polarisation. To overcome this issue without incurring the high computational cost of explicitly polarisable models, we examine the electronic continuum correction (ECC) approach. Specifically, we focus on a charge-scaling variant of ECC that selectively reduces the charges of key molecular groups to account for polarisation effects in a mean-field manner. This strategy enhances the accuracy of charge–charge interactions while preserving compatibility with existing biomolecular force fields and requiring no additional computational overhead. We emphasise the importance of incorporating ECC to achieve more accurate simulations across a range of biologically relevant charged systems, including non-specific interactions, specific binding events, and solution-phase behaviour.

Link for online participation via Zoom:
Meeting ID: 882 4627 9306
Passcode: 663251
Please inform us if you will be participating online or joining our Slack channel
sandhyatiwari@protein.osaka-u.ac.jp, shinobu.ai.prime@osaka-u.ac.jp