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Chemeca 2026 and Hazards Australasia
28 – 30 September, Melbourne, Australia

From Atomistic Molecular Modelling to Shop Floor Synthesis

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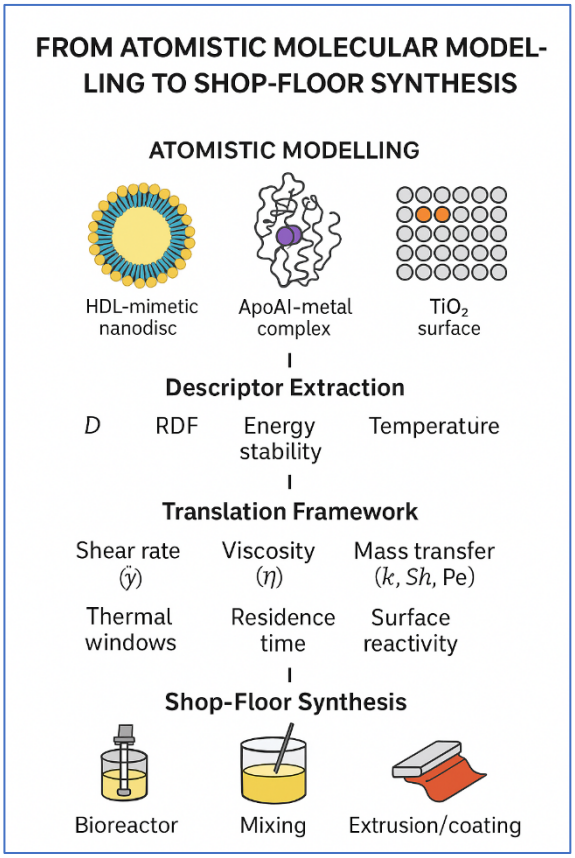
ABSTRACT

Advances in atomistic molecular modelling enable a direct, quantitative bridge between nanoscale behaviour and industrial-scale synthesis. In this work, we demonstrate an integrated framework that translates molecular-level descriptors, diffusion coefficients (D), solvation structure, energetics, and interfacial organisation, into actionable process parameters for manufacturing. Using three representative systems, HDL-mimetic nanodiscs, ApoAI-metal theranostic complexes, and TiO_2-based functional materials, we show how simulation-derived metrics can guide shear-controlled assembly, thermal management, mass-transfer design, and compositional optimisation on the shop floor. For HDL-mimetic nanodiscs, diffusion and O–H radial distribution functions (RDF) predict lipid packing, hydration stability, and shear-sensitive assembly conditions, enabling rational control of size distribution and purity. For ApoAI-metal theranostic constructs, atomistic insights into metal–protein coordination, hydration shells, and energy landscapes inform gentle mixing regimes, ligand stoichiometry, and thermal stability windows essential for preserving biofunctionality. For TiO_2, surface-specific RDFs, adsorption energetics, and interfacial diffusion coefficients translate into scalable synthesis parameters for controlled nucleation, surface functionalisation, and reactor hydrodynamics. Across all systems, we show that nanoscale descriptors can be systematically mapped to macroscopic variables—*shear rate, viscosity, mass-transfer coefficients, residence time, and thermal control*—forming a closed-loop design strategy that unites modelling, synthesis, and scale-up. This nanoscale-to-factory methodology



provides a generalisable pathway for engineering reproducible, high-performance materials and bio-nano systems, enabling predictive manufacturing grounded in molecular physics.

KEY WORDS

Atomistic molecular modelling, Molecular-level descriptors, Nanoscale behaviour, Energetics, Solvation structure, Interfacial organisation, Diffusion coefficients, Interfacial diffusion, Radial distribution functions (RDFs), Adsorption energetics, Bionano systems, Metal–protein coordination, Surface functionalisation, Controlled nucleation, Industrial-scale synthesis, Mass-transfer design, Reactor hydrodynamics, Compositional optimisation.

BIOGRAPHY

Adjunct Professor Michael Akindeju is a distinguished engineering leader whose work spans engineering biology, advanced process design, and innovation in complex industrial systems. He serves as Principal Consultant at MKPro Group, where he delivers high-impact solutions across biotechnology, energy, and manufacturing sectors; and an Adjunct Professor with Federation University, Australia. A Fellow of IChemE and RACI, Chartered Engineer, and Registered Professional Engineer, he is recognised for integrating scientific insight with practical engineering to drive sustainable, technology-enabled transformation. Professor Akindeju is committed to strengthening industry capability, fostering research translation, and mentoring the next generation of engineers through his academic and professional contributions.

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