On the computational methods which may allow to gain insight into microscopic mechanism behind the impact of microplastics on public health

A molecular dynamics case study of biomolecules near nylon nanoparticles

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Environmental and biological context: Nanoplastics from plastic fragmentation are emerging environmental contaminants that can interfere with biological structures and functions at the molecular scale. Evidence indicates perturbations of cell membranes and protein conformations. Prolonged exposure may affect intracellular processes and cause cellular dysfunction, raising concerns about disease processes and public-health risks.

Epidemiological interpretation: Atomistic simulations can provide a molecular-level interpretation of epidemiological findings derived from data-analysis methods.

Computational approach: Molecular dynamics in water to investigate microscopic interactions with proteins and lipid bilayers.

Protein mechanisms to test: Template-mediated peptide adsorption, α-helix to β-sheet-like transitions and β-hairpin unfolding.

Membrane mechanisms to test: Partitioning into hydrophobic cores; possible bilayer thickening, enhanced lipid diffusion and lipid conformational stretching.

Disease relevance: Potential links to aggregation-prone protein misfolding, including processes discussed in prion disorders and Alzheimer's disease.

Exposure-to-mechanism framework: Aquatic food-chain bioaccumulation and human exposure; testing whether chronic low-dose contamination may shift folding landscapes and compromise cellular function.

01 Question & method

Can molecular dynamics distinguish adsorption at the membrane surface from insertion into the hydrophobic core?

Two model systems

A: peptide + nanoplastic in explicit water (NAMD and LAMMPS).

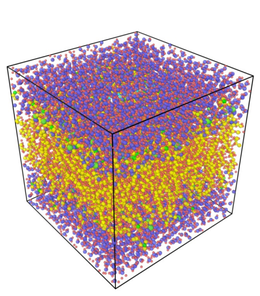
B: nylon oligomer + hydrated DPPC bilayer (LAMMPS).

Simulation workflow

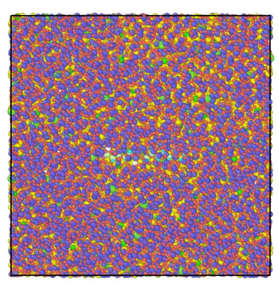
Build and solvate
↓
Minimize energy
↓
Equilibrate
↓
Run production MD
↓
Inspect trajectories

CHARMM-family description for biomolecules; periodic boundaries; semi-isotropic pressure coupling for the membrane setup. Trajectories inspected in VMD and OVITO.

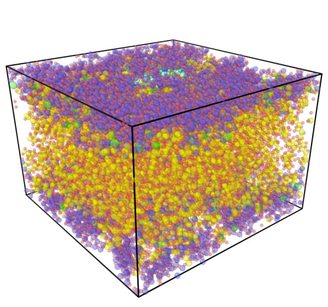
02 What the trajectory shows



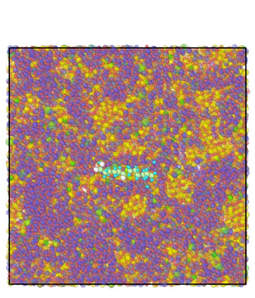
(a) Initial: side view



(b) Initial: top view



(c) 535.25 ps: side view



(d) 535.25 ps: top view

OVITO snapshots from the manuscript (Fig. 2). Initially solvated, the nylon oligomer approaches the hydrated headgroup region during the NPT run (constant particle number, pressure and temperature). DPPC: dipalmitoylphosphatidylcholine.

03 Conclusions

Computational workflow

CHARMM force fields and the dual-engine NAMD/LAMMPS approach support qualitative investigation of nanoplastic-biomolecule interactions in aqueous environments.

Cross-verification and protein mechanisms

Inspection with VMD and OVITO supports consistent identification of interaction patterns, peptide adsorption and secondary-structure perturbations. Nanoplastic-templated helix-to-sheet transitions remain candidate mechanisms.

Nylon at the DPPC interface

Within the simulated timeframe, nylon nanoparticles did not fully enter the hydrophobic bilayer core, but lodged between the hydrophilic headgroups and hydrophobic tails.

Potential membrane consequences

Interfacial positioning suggests possible changes in bilayer thickness, lipid diffusion and permeability, consistent with prior studies of hydrophobic nanoplastics. These effects require quantitative assessment.

Environmental and health implications

The findings suggest a mechanistic link between environmental nanoplastic exposure and altered protein folding landscapes, with potential relevance to diseases associated with conformational changes in biomolecules.

Next steps

Replicated simulations, quantitative analysis and integration with experimental and epidemiological data are needed to establish dose-response relationships and inform mitigation strategies.

04 MD method

Atomic trajectories: MD follows atomic coordinates over time to probe nanoplastic-induced biomolecular perturbations under a force field and explicit environmental conditions.

Classical dynamics: Forces follow the negative potential-energy gradient; numerical integration of Newton’s equations propagates atomic motion.

Periodic boundaries: Replicated simulation boxes approximate bulk conditions at tractable cost; interactions use nearest periodic images under the minimum-image convention.

Thermodynamic control: Thermostats and barostats control temperature and pressure during equilibration and production, targeting the appropriate thermodynamic ensemble.

Selected references

Hollóczki & Gehrke, *ChemPhysChem* 21, 9–12 (2020).
Klauda et al., *J. Phys. Chem. B* 114, 7830–7843 (2010).

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