On the environmental effects of nanoplastics

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Throughout the last decade there has been an increasing scientific and public concern regarding the environmental effects of plastic wastes, especially that of smaller fragmentation products: micro- and nanoplastics. Nanoplastics, with a diameter < 100 nm, have been reported to enter the bodies and organs of animals and humans, but until very recently little was known about the extent of their actual effects. The difficulties of the corresponding research lie in the challenging detection of these small, mostly organic species in colloidal solutions of similarly sized biomolecules.

To tackle these problems, we pioneered the application of molecular modeling and theoretical chemistry for exploring nanoplastic-biomolecule interactions. We found that the presence of these particles may change the structure and dynamics of lipid bilayers, which can have severe effects on the environment and on human health as well [1]. Furthermore, we demonstrated that upon interacting with nanoplastics the secondary structure of proteins can be altered [2]. In the presence of plastic particles, β-loop-like tryptophan zippers show significant changes in the energy demand of cleaving the intramolecular hydrogen bonds that define the structure of these *de novo* proteins. Polyethylene nanoparticles apparently stabilize α-helices, which they also encompass through the rearrangement of the constituting polymer chains. Nylon, on the other hand, spontaneously changes α-helices into a more β-sheet like assembly. Since such changes are responsible for various prion diseases, and have been also related to Alzheimer's disease, these findings are particularly concerning.

Having seen these severely adverse effects it is clear that technological processes are necessary to be developed for the removal of such particles. Considering also the above demonstrated potential of molecular modeling in nanoplastic research, we aimed at designing extractants that can be used for this purpose. The first set of solvents in our focus were hydrophobic ionic liquids. Within these materials, the ions form micelles around the plastics in solution, but do not of disintegrate them into smaller particles. This feature gives ionic liquids a clear advantage over organic molecular solvents such as THF or toluene, in which the disintegration of nanoplastics produces smaller, and potentially more harmful plastic fragments. The interface of ionic liquids and water attracts the polar domain of the former species, since the adjacent water molecules interact stronger with these charged groups than with the non-polar moieties. One might imagine that this structure provides a significant barrier for the phase transfer of the plastic particle, however, as the plastic approaches the interface, the interfacial ions flip over to present their non-polar groups to the particle, allowing the extraction to occur without any activation energy.

Since ionic liquids can be toxic, their use in drinking water and food treatment might be limited to a couple of compounds. For this reason, we extended the scope also to environmentally more benign liquids.

[1] O. Hollóczki, S. Gehrke, *ChemPhysChem* **2020**, *21*, 9-12.
[2] O. Hollóczki, S. Gehrke, *Sci. Rep.* **2019**, *9*, 16013.