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SIMULATIONS OF NANOPLASTICS IN WATER. INTERACTIONS WITH WATER POLLUTANTS

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Abstract. *The ubiquitous presence of micro and nanoplastics (MNPs) in water environments is an emergent environmental problem that has been causing growing concern over the latest years. However, thorough studies on MNP's toxicity and implications for human health are still scarce. Notwithstanding, exposure to MNPs is generally considered as a potential cause of several nefarious effects to human beings, due to their inherent ability to induce intestinal blockage or tissue abrasion. Furthermore, the translocation of MNPs across the gastrointestinal tract to the blood stream may lead to accumulation of particles in the liver, kidneys and gut. Overall, MNPs toxicity may result from the combination of their intrinsic toxicity (e.g., physical damage), their chemical composition (e.g. by leaching of plastic additives), and, as realized more recently, their ability to adsorb trace pollutants (such as heavy metals and organic xenobiotics), accumulate and substantially concentrate them relative to their concentrations in the original aqueous medium, and release them inside the organisms where MNPs are introduced. This latter effect enormously extends the hazardous potential of these pollutant particles. Notably, the tendency of MNPs to aggregate and to adsorb compounds may be related with the par-*

ticles' sizes as well as to their end shapes. The aim of this talk is to show the application of molecular simulations to assess the behavior of three common plastics (polyethylene, polyethylene terephthalate (PET) and the polyamide nylon 6), in different nanoparticle sizes, in the water environment. In addition, interactions of polyethylene with ibuprofen (a pharmaceutical that is a common contaminant of domestic wastewaters and is present as an emergent pollutant in many natural water resources worldwide) are also addressed using the same method. Computer simulations described in this talk consist of the application of the Molecular Dynamics (MD) method, whereby trajectories are sampled in the isothermal-isobaric ensemble as the system's equations of motion are integrated subjected to the ensemble's restrictions, to this end using the velocity-rescaling thermostat and the weak-coupling Berendsen barostat algorithms. Using these MD simulations, a theoretical prediction of the extent of aggregation and average particle sizes of models for the three studied nanoplastics is presented, as well as a discussion of the structure and interactions within the nanoplastic clusters and between these (for the case of polyethylene only) and molecules of the studied pharmaceutical (ibuprofen).