Understanding the adsorption mechanism of organic pollutants on microplastics. A density functional theory study

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Microplastics (MP) are plastic particles smaller than 5 mm in diameter that are mostly made by fragmentation of larger plastic waste. Nowadays, MPa are a very hot topic in the field of environmental sciences. The reason is their occurrence, abundance and wide distribution in the environment and in the food chain. Recently, traces of MP have also been found in human blood, lungs and placenta, proving that they can penetrate tissue and be transported in the organism. The greatest cause for concern is the potentially harmful and toxic effects that MP can have on both the environment and human health. In addition, MP have shown the ability to adsorb and transport coexisting pollutants. The co-contamination of MP with organic pollutants could increase the overall toxicity compared to the toxicity of isolated MP and pollutants. Hence, it is important to understand the adsorption process to properly assess the potential risk of MP. Experimental results to date show that adsorption is physical and mainly governed by weak hydrophobic forces, van der Waals interactions, π-π interactions, electrostatic forces and hydrogen bonds. However, due to the complexity of the system and the many variables controlling the process, the experimental results lack consistency and reproducibility, which makes it impossible to draw clear conclusions and build a predictive model for MP adsorption. Therefore, in our work, we use DFT methods to better understand the individual interactions between organic pollutants and MP. MP is modelled as an oligomer twisted into spherical shapes. The interactions between the model MP and the pollutants are calculated at different adsorption sites to account for the heterogeneity of the MP surface. The results will contribute to a better understanding of the contribution of individual interactions to the adsorption process.

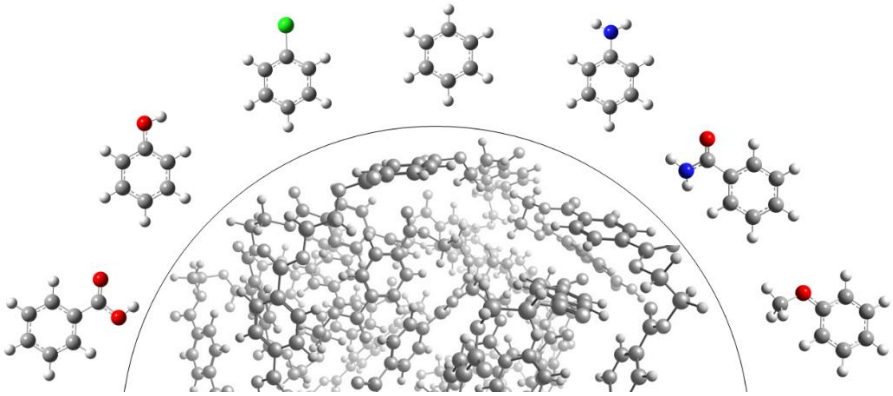

Fig. 1: PET microplastic as a potential carrier of organic pollutants.