

## Chemically tailored graphene for PFAS and other emerging contaminants removal from water

F. Tunioli<sup>[a]</sup>, S. Khaliha<sup>[a]</sup>, L. Favaretto<sup>[a]</sup>, A. Kovtun<sup>[a]</sup>, T.D. Marforio<sup>[b]</sup>, M. Calvaresi<sup>[b]</sup>, V. Palermo<sup>[a,c]</sup>, M. Melucci<sup>[a]</sup>

<sup>[a]</sup>Institute for Organic Synthesis and Photoreactivity (ISOF), National Research Council of Italy (CNR),  
Via P. Gobetti 101, 40129 Bologna, Italy.

<sup>[b]</sup> Alma Mater Studiorum - University of Bologna, Department of Chemistry 'G. Ciamician', via Selmi  
2, 40129 Bologna, Italy.

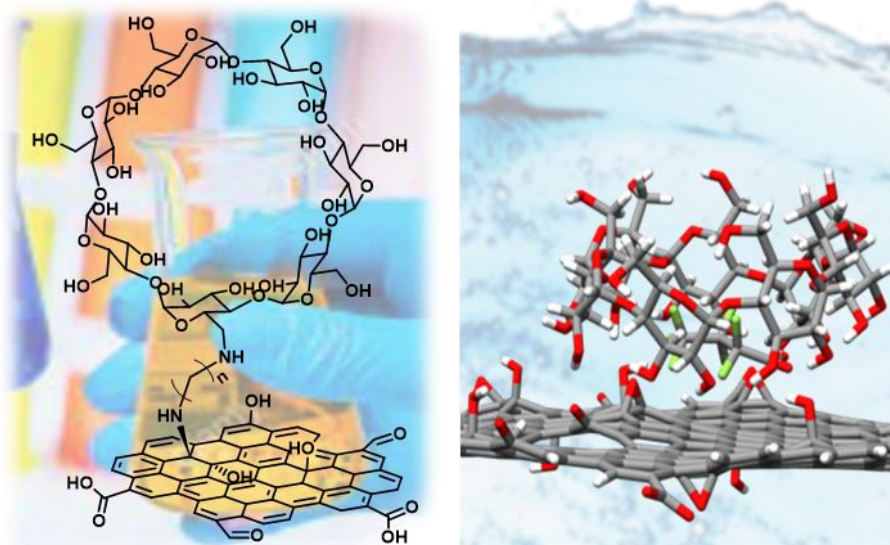
<sup>[c]</sup> Chalmers University of Technology, Chalmersplatsen 4, 41296 Göteborg, Sweden.  
francesca.tunioli@isof.cnr.it

The so called “emerging contaminants” (ECs) (which include pharmaceuticals, cosmetics, pesticides and polyfluoroalkyl substances (PFAS)) are increasingly found in tap water. [1] Graphene based nanomaterials have shown great potential for water purification due to their high surface area and their adsorption properties, promoted by multiple interaction pathways with organic molecules and metal ions. [2], [3] Here, we report on the synthesis of  $\beta$ -cyclodextrine ( $\beta$ -CD) modified graphene oxide (GO) as sorbent with high selectivity and capacity for PFBA, a particularly persistent short chain PFAS. Epoxide ring opening reaction was exploited to bind  $\beta$ -CD to GO, through different sized alkyl spacers. The relationships between alkyl chain length and adsorption capacity is studied by combined adsorption tests and molecular dynamic simulations. The performances have been compared to unmodified GO and other carbon nanomaterials and to those of granular activated carbons, the industrial sorbent benchmark.

### References

- [1] S. Schulze et al., Water Research, 153 (2019) 80-90.
- [2] S. Khaliha et al., FlatChem, 29 (2021) 100283.
- [3] A. Kovtun et al., Faraday Discussions, 227 (2021) 274-290.

### Figure



**Figure 1:**  $\beta$ -cyclodextrine modified graphene oxide (GO- $\beta$ CD) for water remediation.