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Theoretical-computational comparative study of the persistent organic pollutants: adsorption, detection and permeability

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In today's world, the great pollution puzzle is undoubtedly the greatest challenge facing the world's population. Dioxins and dibenzofurans are persistent organic pollutants (POPs); the more toxic forms correspond to their tetrachlorinated derivatives, 2,3,7,8-tetrachloro-p-dibenzodioxin (TCDD) and 2,3,7,8-tetrachlorodibenzofuran (TCDF). The reduction of their emissions, the elimination of pollution already generated and the study of the interaction of these contaminants with living beings are the three fundamental pillars in research related to this particular problem of pollution. In this sense, the computational modelling of these systems ranges from the study of their biological activity to the search for an effective detection method and sustainable treatment.

In this contribution, a complete computational research encompasses: the adsorption of these two "dioxin-like"compounds on new 2D materials, such as white graphene, structurally analogous to graphene but consisting of borazine rings acting more actively as filters or adsorbents, or hybrid boron-nitrogen-carbon (h-BNC) structures; and their subsequent molecular detection using optical spectroscopy, namely, Surface Enhanced Raman Spectroscopy (SERS).

The theoretical work is completed with the study of their behavior in biological media, since the most toxic pollutants accumulate mainly in fatty tissues due to their hydrophobic character. In this way, cell membranes behave as storage reservoirs for pollutants, becoming an internal source of chronic exposure to contamination. Therefore, for a description of the uptake process as well as the changes induced in the membranes at molecular level, the intermolecular interactions between the contaminants and the membranes must be known in detail.

This theoretical research allows for a complete vision of the problem; covering the action, detection and treatment of these substances.

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