Micro-pollutants adsorption through the synthesized carbon: Molecular simulation and experiments

D. Nguemalieu Kouetcha*[1], *H. Ramézani[2],
N. Cohaut[1] , J. Nicolle[1] and C. Vautrin-Ul[1]*

1 Université d'Orléans, ICMN, UMR CNRS 7374, Interfaces, Confinement, Matériaux et Nanostructures, 1b rue de la Férollerie, CS40059, 45071 Orléans cedex, France
2 Ecole Polytechnique de l'Université d'Orléans, Université d'Orléans, ICMN, UMR CNRS 7374, Interfaces, Confinement, Matériaux et Nanostructures, 8 rue Léonard de Vinci, 45072 Orléans, France
daniella.nguemalieu@cnrs-orleans.fr

The advanced technologies are increasingly causing the environmental problems. Consequently, several studies are constantly being made to find the effective way-outs to capture these elements that are dangerous for our environment. In the field of depollution, several methods are applied to deal with these issues, e.g. membrane separation and adsorption [1].

In the current contribution, the main goal is to study the adsorption process of micro-pollutants in aqueous media, following an experimental and numerical approach. However, it should be noted that in order to be able to compare the experimental adsorption with the numerical one, the choice of the structure (adsorbent) on which the adsorption is carried out, is of great importance. Thus, the intercalation of the tetraalkylammonium cations in HOPG electrochemically (Figure1a) enables us to obtain a fairly well organized carbon structure with lamellar porosity in which the experimental adsorption of micro pollutants such as (phenol, biphenol, etc.) could be carried out. Hence, it is possible to determine the experimental adsorption isotherms. By using the numerical approach, the adsorption on a carbon model extracted from a user-written C++ code (Figure1b), is done via the Grand Canonical Monte Carlo method (GCMC). The use of this method is justified by the fact that it allows finding the isosteric heat, density and other relevant parameters of adsorption at the thermodynamic equilibrium state. It can determine the isotherms of numerical adsorptions as well [2]. In this work, we will present at the first stage the way in which the structure can be experimentally obtained to perform the experimental and numerical verifications. At the second stage, the comparison between numerical and experimental outcomes has been provided by means of a user written massively parallel code using MPI paradigm (MPI C++). Lastly, the effect of size and temperature of the adsorption process has been studied including some conclusions and outlooks.

References

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a)

b)
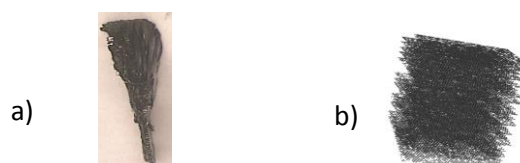
Figure 1: a) TBA intercalation in HOPG and b) Turbostratic carbon extracted from a user written C++ code.