From micro-solvation to solvation: Study of the interaction between pesticide, Ca^{2+} and water

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A large number of pesticides are authorised in the European Union and are used in agriculture. A better understanding of pesticides requires the study of their behaviour and fate in the environment (soil, water and air). This is a major challenge in order to limit their harmful impact on the environment. The global project in which my thesis subject is included follows a step-by-step approach to explore the interactions between a pesticide and the various components of a soil that can be modelled at the atomic scale. Thus, I am studying the micro-hydration[1] of two pesticides, fenhexamid (N-(2,3-dichloro-4-hydroxyphenyl)-1-methylcyclohexanecarboxamid) and metamitron (4-amino-3-methyl-6-phenyl-1,2,4-triazin-5-one), which are respectively a fungicide and an herbicide. Some results and the method used will be presented. First, in molecular dynamics with a DFTB potential, we extensively explore the potential energy surfaces of the Ca^{2+}-pesticide-$(H_2O)_i$ systems for i = 1-20. Along these trajectories, we select n structures that we optimise in DFTB. Among these minima, the m energy-lowest ones are re-optimised in B3LYP/6-311+G(2d,2p) to minimize basis set superposition error. The effects of dispersion are taken into account using the empirical corrections of S. Grimme (D3). In addition, the micro-hydration of the cation and the pesticide are studied through different characteristic energies[2] such as the relative energies of the different minima, the interaction, complexation and deformation energies, giving a better understanding of the micro-hydration of a pesticide interacting with a calcium. The first hydration spheres of the pesticide and the cation are also determined to rationalize the energetical.

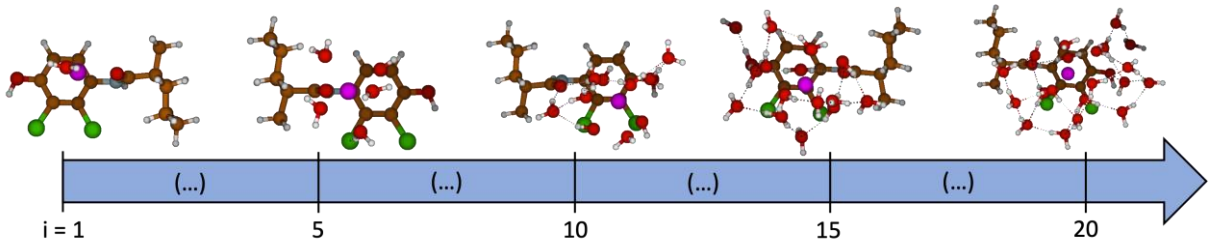

Figure 1. Optimized structure of the lowest-energy isomer for Ca^{2+}-fenhexamid-$(H_2O)_i$ for i= 1, 5, 10, 15 and 20.

Keywords: micro-solvation, pesticide, DFT, DFTB, Molecular Dynamics.

[1] Takis, Panteleimon G. and Papavasileiou, Konstantinos D. and Peristeras, Loukas D. and Melissas, Vasilios S. and Troganis, Anastassios N., Phys. Chem. Chem. Phys., 2013, 15(19), 7354-7362

[2] Campo-Cacharrón, A., Cabaleiro-Lago, E. M., & Rodríguez-Otero, J., Theoretical Chemistry Accounts, (2012), 131, 1-13.