Theoretical Modeling of Ammonia Sensors: Interaction Between Ammonia and Nickel Phthalocyanine

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Organic compounds, such as metallophthalocyanines (MePc), have emerged as important candidates to be used as active materials in numerous applications in Organic Electronics. Several studies have addressed the impact of the position of the central metal atom relative to the organic cage of the phthalocyanine (Pc) and the possibility of exploiting it in numerous applications. Pcs are sensitive to the presence of substances such as carbon dioxide (CO₂) and ammonia (NH₃) [1], for example, which allows the incorporation of this class of molecules in the development of chemical sensors for the identification of such substances. With the population and industrial growth in the last years, the emission of toxic gases in the environment has increased significantly, requiring a greater control of these compounds. In order to simulate how the ammonia sensor works, we extracted a NiPc crystal (nickel phthalocyanine) from the CCDC crystallographic database [2] and we used the *Materials Studio* computational package to add NH₃ molecules to a periodic box. We performed a Molecular Dynamics simulation in the system in order to identify how ammonia interacts with NiPc. We have employed the Density Functional Theory (DFT) to examine the structural, electronic and optical properties of the system. When the Pc molecule is exposed to the ammonia gas, the interaction between the gas and the metal center of the Pc presents a change in its conductivity [1]. The computational calculations indicated the interaction of the ammonia with the metallic center of the Pc, promoting a displacement out of the plane of the central metal (Ni), causing a loss of symmetry [3]. Our results support the hypothesis that the metal serves as a transfer channel between ammonia and NiPc. These data show that NiPc can be designed and used for sensing ammonia. This approach seems to be useful for the development of sensor arrays.

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References:

- [1] Claessens, C. G., Hahn, U., Torres, T. Phthalocyanines: from outstanding electronic properties to emerging applications. *The Chemical Record*. 2008, **8**, 75-97.
- [2] C. R. Groom, I. J. Bruno, M. P. Lightfoot and S. C. Ward, *Acta Cryst.* (2016). B72, 171-179.
- [3] Baggio, A. R., Machado, D. F. S., Silva, V. H. C., Paterno, L. G., Oliveira, C. B. *Physical Chemistry Chemical Physics*. 2017, **19**(17), 10843-10853.