

Adsorption of 5-S-cysteinyl-dopamine on graphene oxide: A possible route for a novel Parkinson's disease biosensor

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5-S-cysteinyl-dopamine (5-S-CysDA) is an endogenous product of dopamine metabolism related with the premature degeneration of dopaminergic neurons in Parkinson's disease (PD) [1]. Early detection of exclusive molecules of PD is highly required in clinics. Graphene and its derivatives, such as graphene oxide (GO) and reduced graphene oxide (rGO) have shown a great potential to adsorb molecules selectively, making them excellent materials for the design of versatile biosensors [2]. By using Raman spectroscopy and DFT computations, along with a QTAIM topological analysis, we studied the chemical adsorption of 5-S-CysDA over GO (CysDA/GO complex) in order to unveil the role of the different intermolecular interactions responsible for the Graphene Enhanced Raman Spectroscopy (GERS) phenomenon in this system [3-4]. It was found that the absorption process allows both, to quench the CysDA intrinsic fluorescence and to enhance its Raman signals, obtaining in this way a clear Raman spectrum of CysDA. From the DFT simulation it is observed that protonation of CysDA favours the interaction with GO. The most relevant contacts stabilizing the complex and enhancing the Raman bands of CysDA are O-H...O and O-H...N. Thus, functionalization of GO with amine groups could increase the selectivity of CysDA, facilitating its detection by means of Raman spectroscopy and serving as a basis for the design of a novel PD biosensor.

Figures

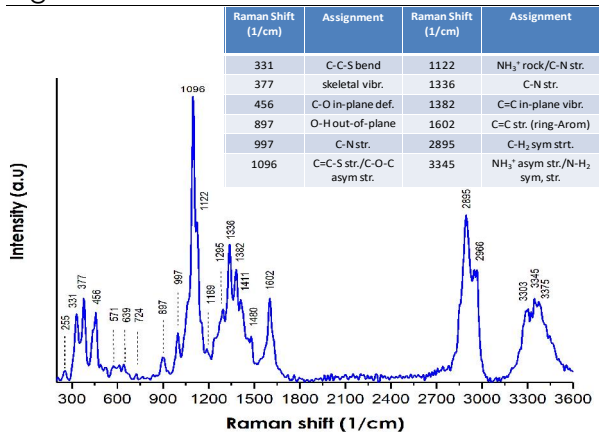


Figure 1: Raman spectra of 5-S-CysDA adsorbed over GO with the main bands assigned.

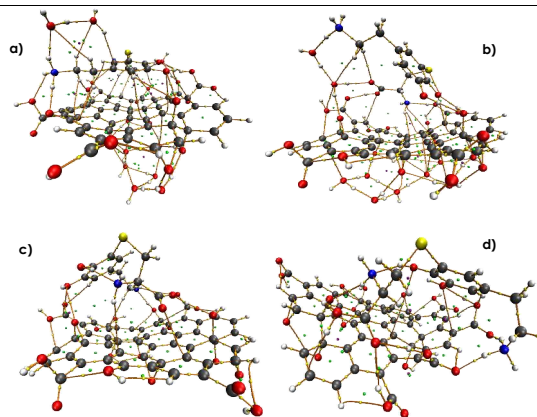


Figure 2: Molecular graphs of some representative arrays of the CysDA/GO complex: a) neutral-hydrated, b) hydrated, c) neutral and d) protonated.

References

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- [2] Zhang, N., et al., *Chemistry of Materials*, 18 (2016) 6426-6435.
- [3] Fu, W., et al., *Advanced Materials*, 6 (2016) 1-25.
- [4] Carballeira, DL., et al., *Physical Chemistry Chemical Physics*, 18 (2016) 15312-1532.