Experimental and Theoretical Insights on the adsorptive properties of Graphene Oxide toward the removal of (2*E*, 5*E*)-2,5-Bis-(2-trifluoromethyl) cyclopentanone

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This study focused on the adsorption of (2E,5E)-2,5-Bis-(2-trifluoromethyl)-cyclopentanone [1] using synthesized graphene oxide as an adsorbent. First, the monocarbonyl compound was synthesized [2], and further underwent purification and structural characterization by FTIR, NMR and MS. Theoretical calculations based on Density Functional Theory (DFT) were conducted and an adsorption mechanism is proposed indicating also the interaction type and evaluating the adsorption energy [3]. Prior to its use, GOx is fully characterized by various spectroscopic methods and used as an adsorbent. The adsorption efficiency and quantity were evaluated via UV-Vis measurements. Furthermore, a comparison with a graphene as an adsorbent of choice was also performed.

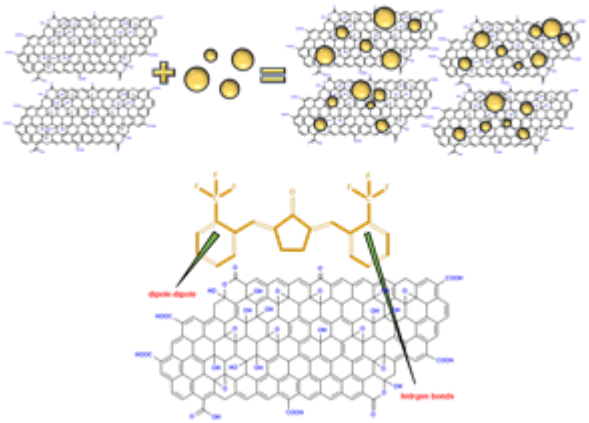

Figure 1: The interaction mechanism between GOx and the yellow color of the compound.

Keywords: MACs; GOx; theoretical calculation; synthesis; characterization.

References

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