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Nanoscale Molecular Surface Electron Localization

In this work we will consider the ability of molecular surfaces at the nanoscale in localizing excess charge. Previously, we have affirmed the design of molecular sheets with hydrogen bonding capacities (from the strategic placement of distributed OH groups) on one side of the surface.

On the opposing side, hydrogen atoms aided in the formation of charge pockets of positive charge that were used to trap excess electrons. We will start from these beginnings to further the aspect of electron localization in fullerenes, nanotubes and graphene sheets based on charge transfer mechanisms with alkali metal atoms. Future prospects from the elucidation of experimental and theoretical approaches will be discussed and correlated to computational limitations.



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