

Modeling of Triplet-Triplet Annihilation on Ionic Liquid systems

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Photon upconversion (UC), converting low-energy photons to higher-energy photons, has attracted much attention because of its potential to overcome the thermodynamic efficiency limits in solar energy conversion devices, including photovoltaic cells and photochemical hydrogen production. Conventional methods, such as multiple-photon absorption require light intensities that are orders of magnitude higher than solar irradiance, and their low conversion efficiencies diminish their appeal. However, an alternative UC mechanism based on the triplet-triplet annihilation developed in the last decade offers numerous advantages over the aforementioned techniques.^[1]

In recent years, Kimizuka *et al.* developed the first example of triplet-triplet annihilation-based photon upconversion (TTA-UC) using chromophoric ionic liquids (ILs) that contain ionic acceptors.^[2]

This study represents an essential step towards the understanding at a molecular level of the bulk structure of these chromophoric ionic liquids (ILs). Molecular Dynamics (MD) simulations were carried out with trihexyl-(tetradecyl) octylphosphonium cation and anthracene-2-sulfonate, 9,10-dimethoxyanthracene-2-sulfonate and 9,10-diphenylanthracene-2-sulfonate anions. The structure of ionic liquids was investigated using the analysis of the structure factor functions, $S(q)$, pair radial distribution functions and the correlation between interaction centers in the anthracene moieties (Fig. 1) that can explain the large efficiency of the electron transfer processes involving the triplet species.^[3]

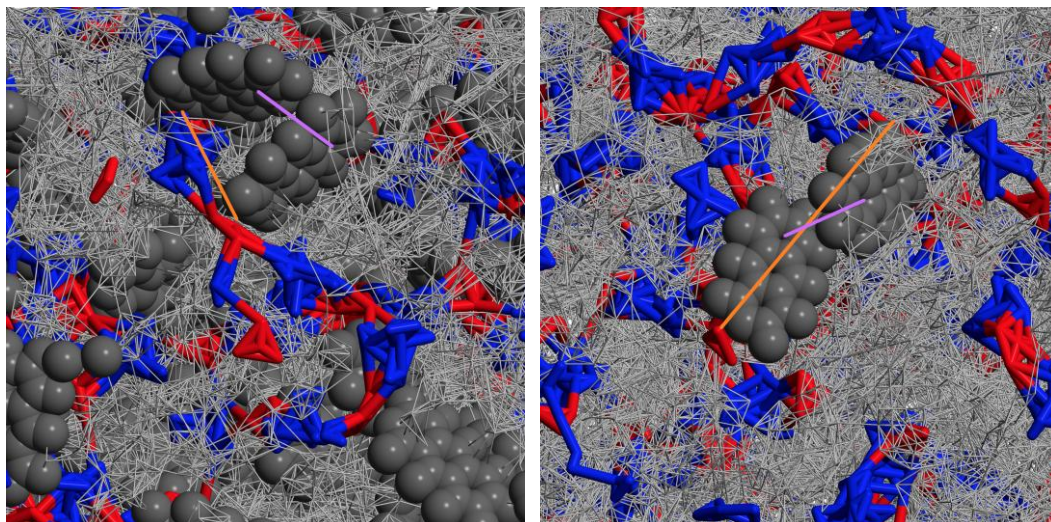


Figure 1. Snapshots of two anthracene moieties anchored to a polar strand at different distances.

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