

# CREM of Photo Induced Charge Separation Mechanisms across Controlled Molecular Spacers

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## Abstract

Thin dielectric spacers are commonly used for the enhancement and real-time control over charge separation mechanisms in various devices. Interesting features in this matter are proposed by self-assembled molecular layers (SAMs), with which fine tuning of the spacer thickness, interfacial binding and intrinsic properties is typically available. On the other hand, the structural and composition integrity of molecular spacers frequently presents critical issues and a challenging demand for simultaneous detection of electrical and structural characteristics.

Specifically for the latter characterization challenge, a promising answer is proposed by the CREM (chemically resolved electrical measurements) technique.[1-3] Based on x-ray photoelectron spectroscopy (XPS), CREM has already demonstrated unique capabilities with which detailed understanding of charge transport processes in heterostructures could be achieved. Within a single experiment, CREM would usually provide the system's composition and its real-time modifications under external stimuli; a measure of the internal fields and band offsets; charge transport data, trapping characteristics and more; all extracted with no top contact and, frequently, at remarkably high sensitivities.

The present work focuses on the transport of hot, photoexcited, charges across organic spacers. Samples consist of molecular layers self-assembled on gold, on top of which CdSe nanoparticles are deposited. Under light illumination, electron-hole pairs are created at the CdSe particles and their transport to the gold through the mediating linker is investigated. The competing mechanisms of electron vs hole transport are found to vary in magnitude as a function of spacer thickness and conjugation degree. In addition, the emergence of defect states and their (sometimes surprising) impact on structural and electrical characteristics are revealed. Deeper insight is proposed by our theoretical study and complementary techniques. Remarkably, the entire set of SAMs can thus be put on a common ruler that governs leading factors in the transport problem.

## References

1. H. Cohen, *Appl. Phys. Lett.* **85**, 1271 (2004).
2. N. Filip-Granit et al., *Nano Lett.* **6**, 2848 (2006).
3. Elad D. Mentovich et al., *J. Am. Chem. Soc.* **134**, 8468-73 (2012).

## Supplementary Page

Simulated photo-induced surface charge ( $Q$ ) and photoluminescence intensity (PL) as a function of the hole-transport rate parameter ( $k_h$ ). The figure exemplifies, in agreement with the experimental results, the roles of molecular length and conjugation and, in particular, the crossover between regimes where PL and  $Q$  can adopt either opposite or common trends. Guidelines for device optimization can thus be drawn.

