

Ultraviolet Absorption and Transient Photocurrent Spectroscopy in Organic Thin Layers as Evidence of Super Atomic Molecular Orbitals in Corannulene

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Abstract

Distortion of sp_2 carbon orbitals in curved π -conjugated molecule of corannulene induces a set of extensive molecular orbitals - super atomic molecular orbitals (SAMOs). Due to their extent and overlap, they could potentially play a key role in the charge transport mechanism of future devices. Similar behaviour is expected in other curved sp_2 carbons like fullerene or sumanene. However experimental evidence of charge transport through SAMOs in these materials is hindered, because the energy of the lowest SAMO is above LUMO. Hence SAMO can be populated only for a fragment of time before the charge relaxes to LUMO. We achieved to populate SAMO using a short light pulse and measured transient photoconductivity response, which occurred within several nanoseconds. Comparing transient photocurrent spectra with optical absorption in thin layers, the photocurrent shows a rise over an energy region where the optical absorption is decreasing but where SAMOs are predicted to contribute to photoexcitation (Figure 1). This photocurrent behaviour can only be interpreted as a signature of the SAMO-

mediated electron transport, in a region where low absorption of photons is compensated by significant enhancement of electron transport through diffuse SAMOs. Through a combination of experimental optical (solution phase and thin films) and photoconductivity spectra of corannulene thin films with supportive GW-BSE theoretical predictions, evidence for diffuse super atomic molecular orbitals (SAMOs) in corannulene is established.

References

- [1] N. Pastukhova, L. Martin Samos, L. Zoppi, E. Pavlica, J. Mathew, G. Bratina, J. S. Siegel, and K. K. Baldrige, Evidence of enhanced photocurrent response in corannulene films, RSC Advances, 2017,7, 45601-45606.

Figures

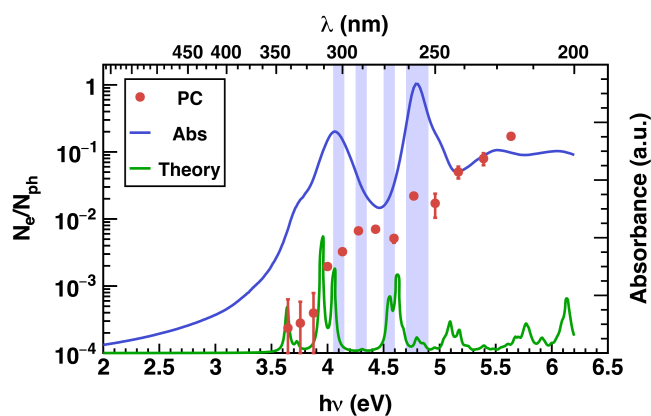


Figure 1: Comparison of the measured absorption (Abs) of corannulene in spin-coated thin film (blue), transient photoconductivity (PC) of corannulene thin layer (red spots) and theoretical absorption (green); regions with SAMO contributions are highlighted in violet.