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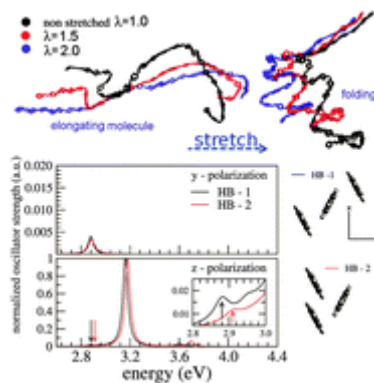
Physical Chemistry Chemical Physics

Polarized emission from stretched PPV films viewed at the molecular level

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Abstract

We present a study on the photoluminescence (PL) of thin films of poly-(*p*-phenylene vinylene) (PPV), non-stretched and uniaxially stretched. The experimental study was carried out using linear polarized light as the excitation beam, oriented either parallel or perpendicular to the stretch axis (*S*). The results showed that when the excitation light source has polarization perpendicularly oriented to the stretch direction, the emitted PL presents maximum intensity in the orientation *S*, and a minimum in the direction orthogonal to *S*. In order to understand this interesting phenomenon, we employ theoretical simulations at the atomistic level. We use classical molecular dynamics to simulate amorphous PPV films, non-stretched and stretched, from which we find a tendency of overall alignment of PV units to *S*, and of local clustering in herring-bone and π -stacking partial symmetries. Our study of optical activity of these kinds of clusters, performed through a quantum semi-empirical method, allows us to explain this polarization conversion behavior, and indicates the possibility of using underivatized PPV as the active layer for polarized electroluminescent devices.

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Article information

<https://doi.org/10.1039/C5CP02513C>

Article type

Paper

Submitted

29 Apr 2015

Accepted

05 Jul 2015

First published

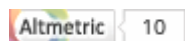
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Citation*Phys. Chem. Chem. Phys.*, 2015, **17**, 20530-20536

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