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Molecular dynamics of conjugated polymers and its influence on organic solar cell performance

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Conjugated polymers are the main components of a new generation of organic optoelectronic devices, of which organic solar cells are the most promising ones. A summary of quasielastic neutron scattering experiments carried out on P3HT, P3OT and the low band-gap PCPDTBT conjugated polymers during the past few years on different backscattering spectrometers, both on ILL (IN10, IN16 and IN16B) as well as on ISIS (IRIS, OSIRIS in time-of-flight mode) will be presented. Both quasielastic and elastic scattering experiments have been performed, and a discussion on fitting models and their ability to explain the molecular dynamics (and structure) of the polymers will be discussed. The new capabilities offered by IN16B, such as inelastic fixed window scans will also be presented.
The polymers, acting as electron donors upon light excitation and mixed with electron acceptors such as fullerene derivatives, create a "bulk heterojunction"which is the core of fully operational organic solar cells. The performance of the cells is related to the polymer dynamics at different temperatures, and only the combination of neutron scattering and I-V electronic measurements will provide sufficient information to improve future mixtures and fabrication procedures for more efficient and stable solar cells.

Primary author: Dr URBINA, Antonio (Technical University of Cartagena, UPCT)

Co-authors: Dr DIAZ-PANIAGUA, Carlos (Instituto de Ciencia de Materiales de Madrid-CSIC); Prof. BATALLAN, Francisco (Instituto de Ciencia de Materiales de Madrid-CSIC); Dr ABAD, Jose (Technical University of Cartagena); Dr SEYDEL, Tilo (Institut Max von Laue - Paul Langevin); Dr GARCIA SAKAI, Victoria (ISIS Neutron and Muon Source, STFC)

Presenter: Dr URBINA, Antonio (Technical University of Cartagena, UPCT)

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