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Structure and dynamics of conjugated polymers from scattering and simulations

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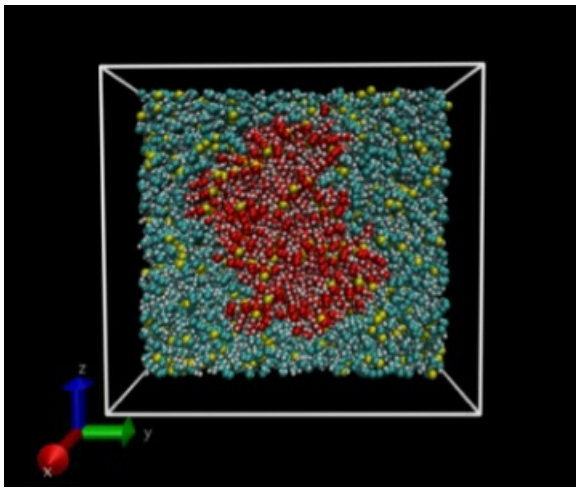
Conjugated polymer films, nanofibers, and networks can be ideal materials for the design of efficient photovoltaic devices, batteries, thermoelectric cells, light emitting diodes and many emerging technologies.[1] It is also recognized that the structure and dynamics of organic semiconductor materials correlates strongly with large changes in optical, electronic and mechanical properties so that their control and manipulation is essential to advancing the field. This presentation outlines the use of neutron scattering techniques in the development of structure-property relationships for conjugated polymer nano materials.[2] It also highlights recent results on the use of neutron and x-ray scattering techniques for the development of improved molecular simulation force fields and structural parameters specifically produced for conjugated polymers. Quasi-elastic neutron scattering (QENS) experiments are used along with computationally efficient MD simulations to understand the nature of important nanoscale motions. X-ray and polarized neutron diffraction are also used to correlate experimental and model-generated polymer structures. QENS validation of MD force fields presents a unique opportunity to increase the accuracy of highly uncertain parameters used in simulation of conjugated polymers such as partial charges and backbone torsion. These parameters are currently estimated from quantum mechanical calculations such as density functional theory but, unlike many force fields for small molecules, are not parameterized with available experimental data. High variability is observed in these parameters for the small number of force fields that have been proposed in the literature. A vision for the accelerated development of accurate force fields for these classes of materials is also proposed.

[1] Newbloom G., de la Iglesia P., Pozzo L., (2014), Soft matter 10, 8945
[2] Newbloom G., Hoffmann S., West A., Gile M., Sista P., Cheung H., Pfaendtner J., Pozzo L. (2015), Langmuir, 31, 458



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