The effect of isotope substitution on stability and dynamics of polymers

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It is increasingly recognized that properties of polymers can be affected by nuclear quantum effects and related isotopic substitution[1]. We investigate isotopic effects of deuterium substitution on the properties of selected polymers. The effects of selective deuterium isotope substitution on poly(3-hexylthiophene) (P3HT) chain stacking is studied experimentally by X-ray diffraction (XRD) in combination with gel permeation chromatography and theoretically by density functional theory, quantum molecular dynamics, discrete variable representation of nuclear wave functions and perturbation theory. For four P3HT materials with different levels and position for selective deuteration (pristine, main-chain deuterated, side-chain deuterated, and fully deuterated), the XRD measurements show that main-chain thiophene deuteration significantly reduces crystallinity, regardless of the side-chain deuteration[2]. We discuss how the quantum nuclear effects modulate the crystal stability, dynamics and properties of polymers.

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[2] J. Phys. Chem. Lett., 8, 4333 (2017)