

# Micro-structure and dynamics of polymers: lessons learned from inelastic neutron scattering (INS) and periodic-DFT calculations

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The main strategy to delve deeper into the structure-property correlations in polymeric materials takes advantage of inelastic neutron scattering (INS) combined with discrete and periodic DFT calculations [1-3]. This combination is ideal either to assist the elucidation of measured data or, conversely, as method of validating theoretical models. In particular, the synergy between INS and periodic-DFT calculations allowed the reliable assignment of INS bands to vibrational modes of crystalline polymer forms (Figure 1). This work aimed at the characterization of polymer structure and dynamics. These embraces both natural polymers (e.g. cellulose and bacterial cellulose) and bio-based synthetic polymers (furanidicaboxylate polyesters).

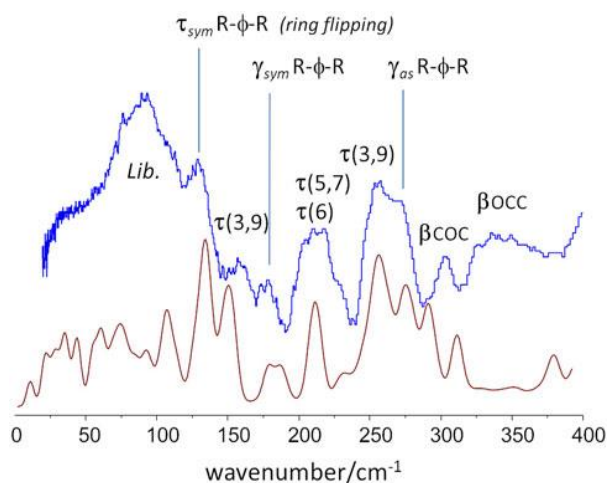


Fig.1- Low-wavenumber region of the INS spectra of poly(butylene 2,5-furandicarboxylate: experimental (top, blue) and calculated (bottom, red) for the *aa-gtg* crystal model

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## References

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