MS19-O5 Lattice dynamics of the ionic superconductor Li_4C_{60}. Inelastic neutron scattering and Powder Averaged Lattice Dynamics (PALD) investigations.

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The two-dimensional polymer structure and lattice dynamics of the superionic conductor Li_4C_{60} (ionic conductivity of 10^{-2} S/cm at room temperature [1]), are investigated by neutron diffraction and neutron spectroscopy. The peculiar bonding architecture of this compound is confirmed through the precise localization of the carbon atoms involved in the intermolecular bonds. The spectral features of this phase are revealed through a combination of *ab initio* lattice dynamics calculations and inelastic neutron scattering experiments. The neutron scattering observables are found to be in excellent agreement with the simulations, the latter predicting a partial charge transfer from the Li atoms to the C_{60} cage. The absence of a well-defined band associated with the Li atoms in the experimental spectrum suggests that this species is not ordered even at the lowest temperatures. The calculations also predict an unstable Li sublattice at a temperature of ~200 K, which we relate to the large ionic diffusivity of this system : low-frequency optic modes of the Li ions couple to the soft structure of the polymer [2].

[1] M. Ricco et al., Phys. Rev. Lett., **102** (2009) 145901.

[2] S. Rols et al. Phys. Rev. B, **92** (2015) 014305

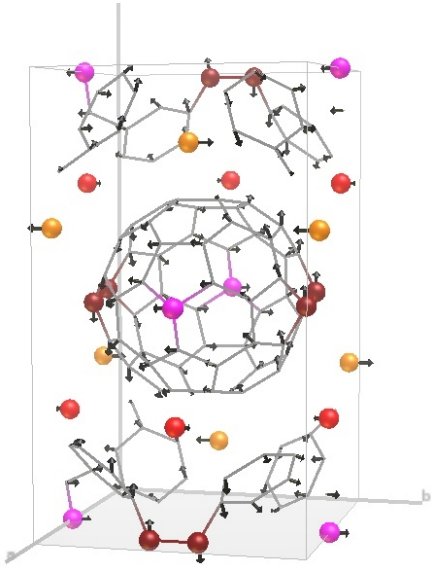

Figure 1. Optic low frequency hybrid mode, involving C_{60} deformation and Li translations.

Keywords: superionic conductor, inelastic neutron scattering, fullerides, DFT