Electronic supplementary information for "Probing the thermal stability and decomposition mechanism of a magnesium-fullerene polymer via X-ray Raman spectroscopy, X-ray diffraction and molecular dynamics simulations"†

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Fig. S1 Selected region of the Raman spectrum of the Mg₂C₆₀ sample treated at 700°C.

Figure S1 reports a selected region of the Raman spectrum of the sample treated at 700°C.

The spectrum can be clearly attributed to intercalated fullerene compounds, and shows the emergence of typical Hg(7) and Ag(2) Raman lines at 1426 and 1457 cm⁻¹, respectively. An empirical rule based on existing literature states that the latter is shifted to lower wavenumbers by 6–7 cm⁻¹ for every electron transferred to C₆₀ and 5 cm⁻¹ per polymer bond due to the softening of the bond stretching modes as the electrons occupy the antibonding molecular orbitals. The shift of Ag(2) mode with respect to its energy in pristine C₆₀ (1469 cm⁻¹) suggests a charge transfer close to 2 electrons and is in agreement with the picture of intercalated magnesium suggested by X-ray Raman scattering.

References