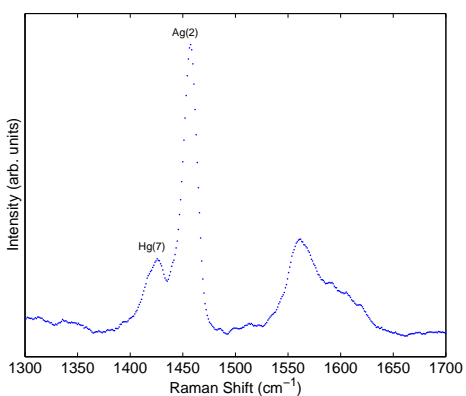


Cite this: DOI: 10.1039/xxxxxxxxxx

## 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"<sup>†</sup>

Matteo Aramini,<sup>\*a</sup> Johannes Niskanen,<sup>a</sup> Chiara Cavallari,<sup>b,c</sup> Daniele Pontiroli,<sup>c</sup> Abdurrahman Musazay,<sup>a</sup> Michael Krisch,<sup>d</sup> Mikko Hakala<sup>a</sup> Simo Huotari<sup>\*a</sup>



**Fig. S1** Selected region of the Raman spectrum of the Mg<sub>2</sub>C<sub>60</sub> 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<sup>-1</sup>, respectively<sup>1</sup>. An empirical rule based on existing literature states that the latter is shifted to

lower wavenumbers by 6-7 cm<sup>-1</sup> for every electron transferred to C<sub>60</sub> and 5 cm<sup>-1</sup> per polymer bond<sup>2</sup> 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 C<sub>60</sub> (1469 cm<sup>-1</sup>) suggests a charge transfer close to 2 electrons and is in agreement with the picture of

<sup>a</sup> Department of Physics, University of Helsinki, Gustav Hällströmin katu 2, P.O. Box 64 00014 Helsinki, Finland; Corresponding authors: Tel +358(0)2941-50638, E-mail address; matteo.aramini@helsinki.fi, E-mail address; simo.huotari@helsinki.fi

<sup>b</sup> Institut Laue Langevin, BP 156, 71 Avenue des Martyrs, 38000, Grenoble, France

<sup>c</sup> Dipartimento di Fisica e Scienze della Terra, Università degli studi di Parma, Viale delle Scienze 7/a, 43124 Parma, Italy

<sup>d</sup> European Synchrotron Radiation Facility, BP 220, 71 Avenue des Martyrs, 38000, Grenoble, France

intercalated magnesium suggested by X-ray Raman scattering.

## References

- 1 Z. Dong, P. Zhou, J. Holden, P. Eklund, M. Dresselhaus and G. Dresselhaus, *Phys. Rev. B*,, 1993, **48**, 2862–65.
- 2 T. Wagberg, P. Stenmark and B. Sundqvist, *J. Phys. Chem. Solids*,, 2004, **65**, 317–20.