ESRF	**Experiment title:** Non-adiabatic effects and electron-phonon coupling in LiC_6	**Experiment number**: HS-4393
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Report:

Introduction

Thanks to the recent discovery of graphene, the study of the electronic properties of doped graphene systems has become an intensively studied topic, with both theoretical and experiment studies providing valuable new insights. Experimental techniques which study bulk materials, such as inelastic x-ray scattering (IXS), are unfortunately not always the ideal probe for developing our understanding of these inherently two-dimensional materials. However the graphite intercalation compounds (GICs) can give us a unique insight into the properties of doped graphene, as in many cases the role of the intercalant can be understood as simply acting to dope the graphene layers with electrons. Moreover, the discovery of superconductivity in GICs [1] (T_c up to 11.5 K) raises the inevitable question: can we make graphene superconducting? While it is generally agreed that the superconductivity observed in GICs is due to conventional electron-phonon (e-ph) coupling [2], there is still much controversy over which electrons and which phonons are primarily involved in the e-ph coupling which leads to superconductivity. In this experiment at ID28 we performed meV-resolution IXS measurements of the high-energy graphitic phonons in non-superconducting LiC_6 across the Brillouin zone, our primary aim being to understand e-ph interactions over the whole of reciprocal space.

Experimental Details:

LiC_6 samples were synthesized by immersing large platelets (diameter ~ 5 mm) of single-crystal graphite in molten lithium metal for several days. These samples were transferred into a high purity glove box and loaded into a beryllium dome at the ESRF, which was sealed using indium wire. The very high sample purity was confirmed using diffraction on ID28. The high-energy in-plane graphitic phonons in LiC_6 were measured throughout the (HK0) plane in reciprocal space.

Results:
Fig. 1 shows 9 energy scans measured simultaneously at ID28 at 9 different momentum transfers within the (HK0) plane of LiC_6. The coloured lines are IXS spectra calculated from dynamical matrices produced from of density functional theory (DFT) calculations [3], after convolution with Lorentzians of full-width half-maximum (FWHM) of 0.1 meV (red) and 3.0 meV (blue). The intensities of the phonons in theory and experiment show good agreement, which shows that the phonon eigenvectors are reproduced well by the theory. The phonon energies are not as well reproduced by the theory, but subsequent DFT calculations (not shown here) show even better agreement after the experimentally determined lattice parameters are used in the calculation. In the simulations shown below, the dynamical matrices were calculated using lattice parameters found by energy minimisation within the DFT calculation. We are currently comparing our data in detail to the calculation, not only in the phonon eigenvectors (intensities) and eigenvalues (energies) but also in the e-ph coupling (linewidths).

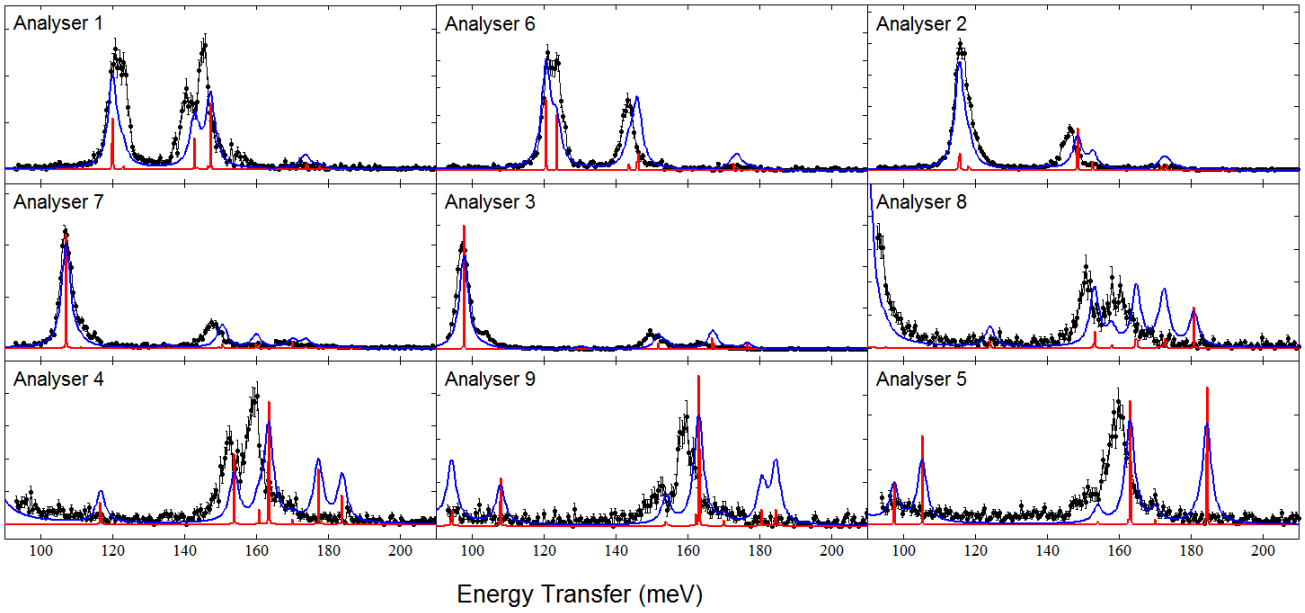

Fig. 1: Here 9 energy scans performed simultaneously on LiC_6 at 9 different momenta are presented, together with the results of DFT calculations for these 9 momenta (red line: DFT simulation after convolution with a Lorentzian of full-width half-maximum (FWHM) of 0.1 meV; blue line: after convolution with Lorentzian of FWHM of 3 meV. These measurements were done with the Si (999) reflection at ID28, leading to an experimental energy resolution of approximately 3 meV

In the inelastic scattering of phonons, the e-ph coupling contribution to the phonon linewidth $\gamma_{\boldsymbol{q}\nu}$ for mode ν with wavevector $\boldsymbol{q}$ and energy $\omega_{\boldsymbol{q}\nu}$ can be related to the electronic density of states at the Fermi level $N(0) \approx$ 0.6 states/(cell eV spin) and the electron-phonon coupling constant $\lambda_{\boldsymbol{q}\nu}$ through the Allen formula [4]

$$\gamma_{q\nu} = 2\pi N(0)\omega_{q\nu}^2 \lambda_{q\nu}$$

We have performed the first measurements of the high-energy phonons in LiC_6. Our detailed phonon linewidth analysis, currently in progress, should allow a detailed measurement of the electron-phonon coupling as a function of $\boldsymbol{q}$ and as a function of the different phonon modes, with significant implications for the physics of doped graphitic systems.

References:

[1] T. E. Weller et al., Nat. Phys. **1**, 39 (2005)
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[3] G. Profeta et al., Nat. Phys. **8**,131 (2012)
[4] P. B. Allen, Phys. Rev. B **6**, 2577 (1972); P. B. Allen and R. Silberglitt, Phys. Rev. B **9**, 4733 (1974)