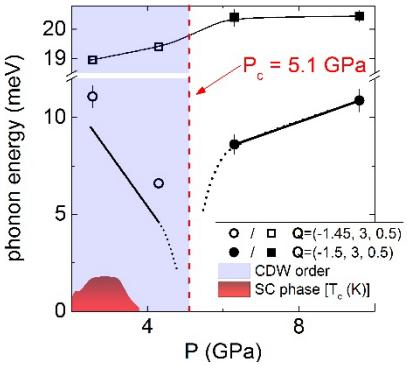
High pressure, anomalous line shapes and precision phonon spectroscopy using inelastic x-ray scattering

Momentum-resolved phonon spectroscopy, traditionally the domain of inelastic neutron scattering, has tremendously benefitted from the development of inelastic x-ray scattering with energy resolution of down to 1 *milli-electronvolt*. Tiny single crystals weighing only few milligrams can now be routinely investigated.

After a short comparison of state-of-the-art inelastic x-ray and neutron scattering experiments, I will review work based on high energy resolution inelastic x-ray scattering focusing on the competition between superconductivity and charge-density-wave (CDW) formation in transition-metal dichalcogenides, namely, *1T*-$TiSe_2$ (Refs. [1,2]) and *2H*-$NbSe_2$ (Ref. [3-5]):

(1) In a high-pressure – low-temperature study of *1T*-$TiSe_2$ we investigated the soft phonon mode of the CDW transition up to nearly 10 GPa and down to 5 K as well as for intercalated Cu_xTiSe_2 at ambient pressure. We find that the intercalation-induced superconductivity can be explained by a solely phonon-mediated pairing mechanism, while this is not possible for the superconducting phase under pressure. We argue that a hybridization of phonon and exciton modes in the pairing mechanism is necessary to explain the full observed temperature-pressure-intercalation phase diagram. These results indicate that *1T*-$TiSe_2$ under pressure is close to the elusive state of the excitonic insulator.



Pressure-dependence of phonon energies in *1T*-$TiSe_2$ under pressure.

(2) *2H*-$NbSe_2$ is one of the few compounds where CDW order and superconductivity co-exist without doping or other tuning parameters. We observe changes of the phonon line shape that are characteristic for systems with strong electron-phonon coupling in the presence of a superconducting energy gap $2\Delta_c$ and from which we can demonstrate an *l* dependence of the superconducting gap. Reversely, our data imply that the CDW energy gap is strongly localized along the *l* direction. This conclusion is corroborated by recent soft x-ray angle-resolved photoemission spectroscopy revealing the 3D Fermi surface of *2H*-$NbSe_2$. The confinement of the CDW gap to a very small momentum region explains the rather low competition and easy coexistence of CDW order and superconductivity in *2H*-$NbSe_2$.

1 Maschek, M. *et al.* Superconductivity and hybrid soft modes in 1T-$TiSe_2$. *Physical Review B* **94**, 214507 (2016).

2 Weber, F. *et al.* Electron-Phonon Coupling and the Soft Phonon Mode in $TiSe_2$. *Physical Review Letters* **107**, 266401 (2011).

3 Weber, F., Rosenkranz, S., Heid, R. & Said, A. H. Superconducting energy gap of 2H−$NbSe_2$ in phonon spectroscopy. *Physical Review B* **94**, 140504(R) (2016).

4 Weber, F. *et al.* Optical phonons and the soft mode in 2H-$NbSe_2$. *Physical Review B* **87**, 245111 (2013).

5 Weber, F. *et al.* Extended Phonon Collapse and the Origin of the Charge-Density Wave in 2H-$NbSe_2$. *Physical Review Letters* **107**, 107403 (2011).