



Institut de Minéralogie et de Physique des Milieux Condensés  
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# SÉMINAIRE

## Lundi 21 novembre, 10h30

Salle de Conférence, 4<sup>ème</sup> étage, Tour 22-23, Salle 1  
IMPMC, Université P. et M. Curie, 4, Place Jussieu, 75005 Paris

### Frank WEBER

Karlsruher Institut für Technologie Institut für Festkörperphysik  
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## PHONON SOFTENING AND CHARGE DENSITY WAVE FORMATION IN NbSe<sub>2</sub> AND TiSe<sub>2</sub>

We report [1] inelastic x-ray scattering measurements of the temperature dependence of phonon dispersion in the prototypical charge-density-wave (CDW) compounds NbSe<sub>2</sub> and TiSe<sub>2</sub>. Surprisingly, acoustic phonons in NbSe<sub>2</sub> soften to zero frequency and become overdamped over an extended region around the CDW wavevector. This extended phonon collapse is dramatically different from the sharp cusp in the phonon dispersion expected from Fermi surface nesting. Instead, our experiments combined with *ab initio* calculations, show that it is the wavevector dependence of the electron-phonon coupling that drives the CDW formation in NbSe<sub>2</sub> and determines its periodicity. For TiSe<sub>2</sub> [2], we found theoretically that the above described electron-phonon coupling scenario is able to stabilize a CDW ground state as well. Calculations of the lattice dynamical properties are in good agreement with our experimental results for the soft phonon dispersion and linewidth. A more detailed analysis of the calculations yield wavevector dependent matrix elements, strong enough to stabilize the CDW order in combination with an enhanced electronic joint density of states at the ordering wavevector.

<sup>1</sup> F. Weber *et al.*, *Physical Review Letters* 107 (10), 107403 (2011).

<sup>2</sup> F. Weber, *et al.* <http://arXiv.org/abs/1105.3292> (2011).