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Soft Phonons in CDW Phase Transitions from first principles

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Motivation

Structural phase transitions and anomalous lattice dynamics properties are often interrelated. Charge-density wave (CDW) transitions are typically accompanied by the presence of soft phonons, which become unstable at the transition temperature. DFT based linear-response techniques provide insight into the soft-mode properties and the underlying mechanism driving the CDW phase transition.

Approach

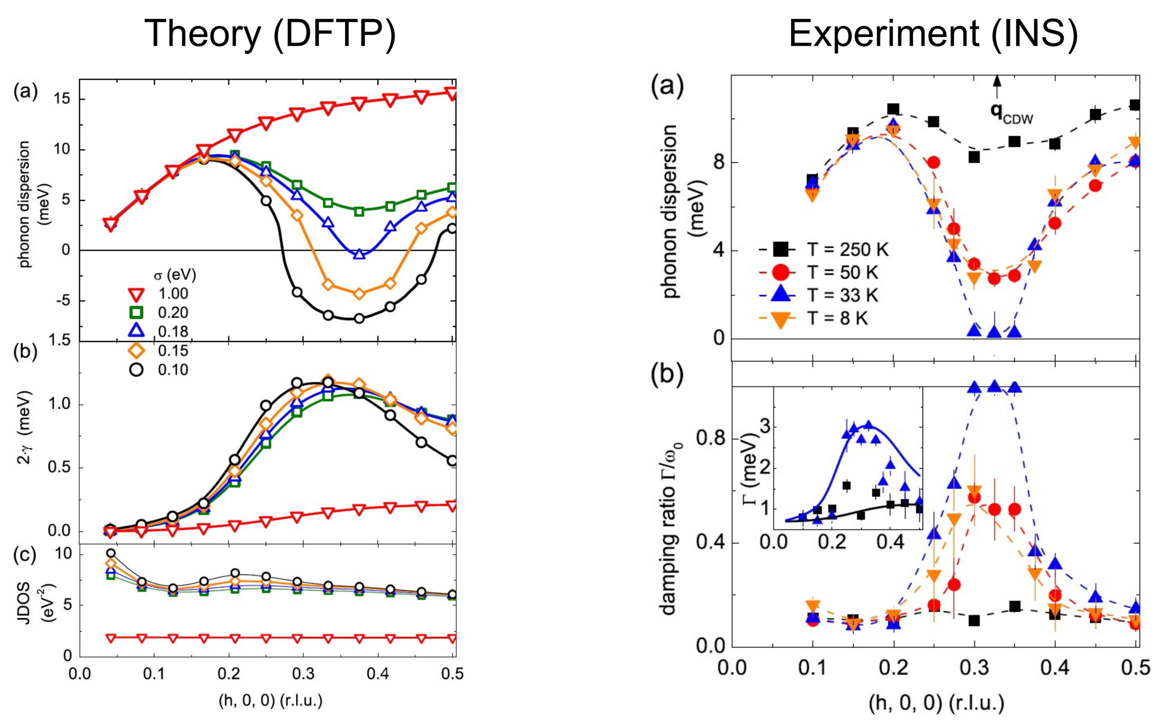
- Density functional perturbation theory, implemented in the mixed-basis pseudopotential method [1,2]
- Provides phonon dispersion without phenomenological parameters and full momentum structure of the electron-phonon coupling (EPC) matrix elements $g(k, k+q)$

Key quantities

- Phonon linewidth: $\gamma(q) = 2\pi\omega_q \sum_k |g(k,k+q)|^2 \delta(\varepsilon_k)\delta(\varepsilon_{k+q})$
- Joint density of states: $\mathrm{JDOS}(q) = \sum_k \delta(\varepsilon_k)\delta(\varepsilon_{k+q})$

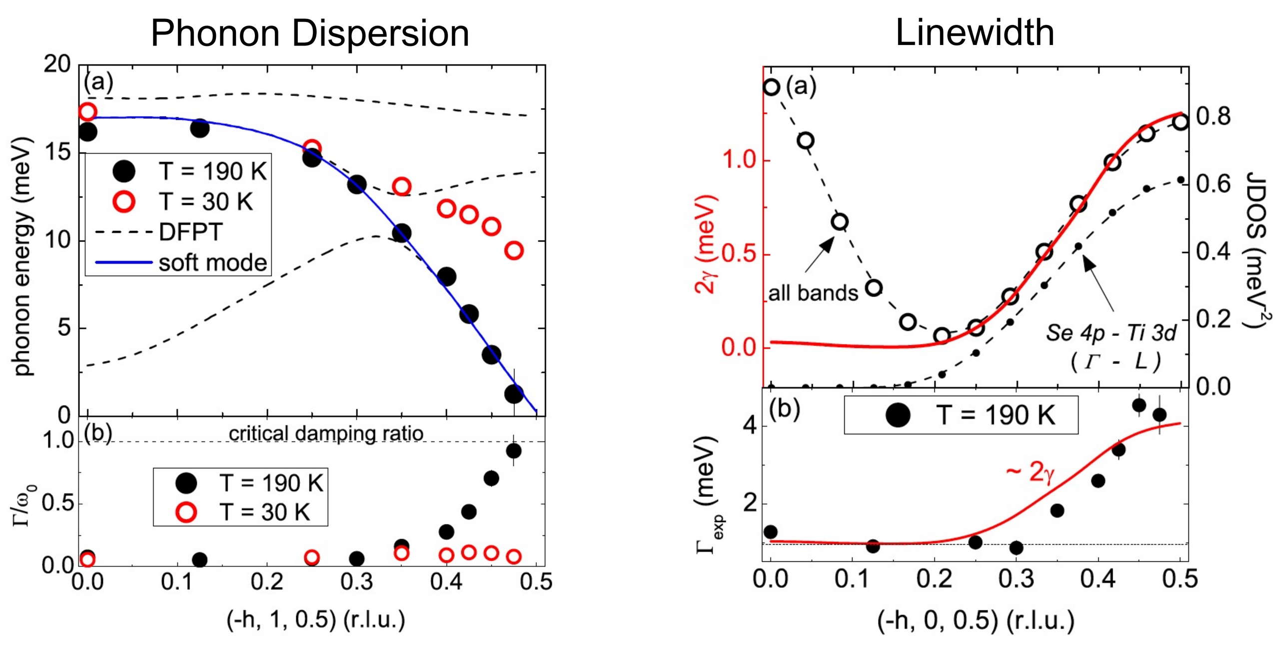
TM Dichalcogenides

2H-NbSe$_2$ [3]: T_{CDW}=33 K, Q_c=(0.329,0,0)



- Extended momentum range of soft modes
- Enhanced EPC near critical wavevector Q_c
- No enhanced JDOS -> No Fermi surface nesting
- Q_c determined by momentum dependence of EPC

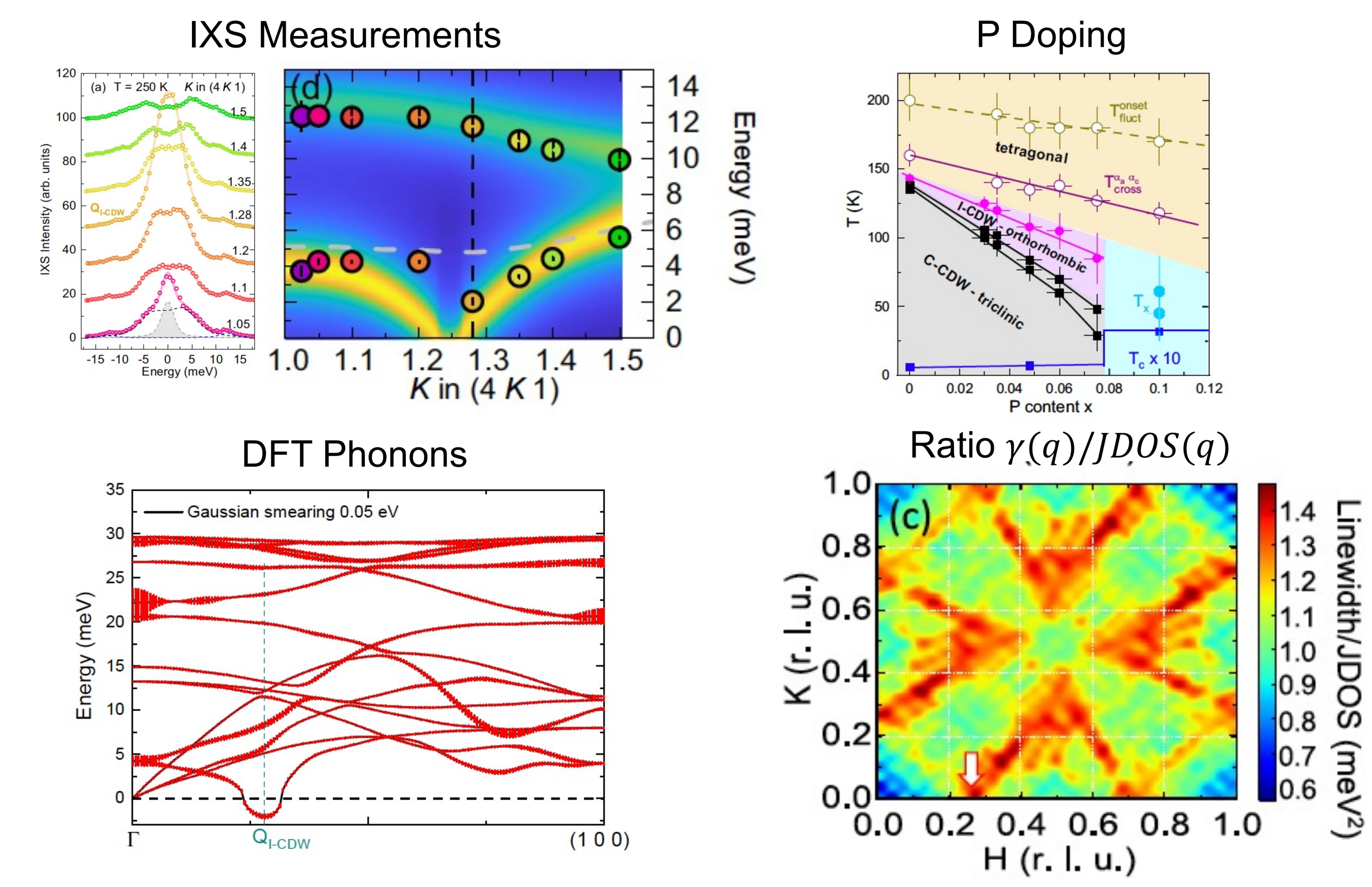
1T-TiSe$_2$ [4]: T_{CDW}=200 K, Q_c=(0.5,0,0.5)



- Commensurate CDW; soft mode at BZ boundary
- Critical wavevector Q_c determined by Fermi surface nesting
- Excitonic insulator?

Ni-based Arsenides

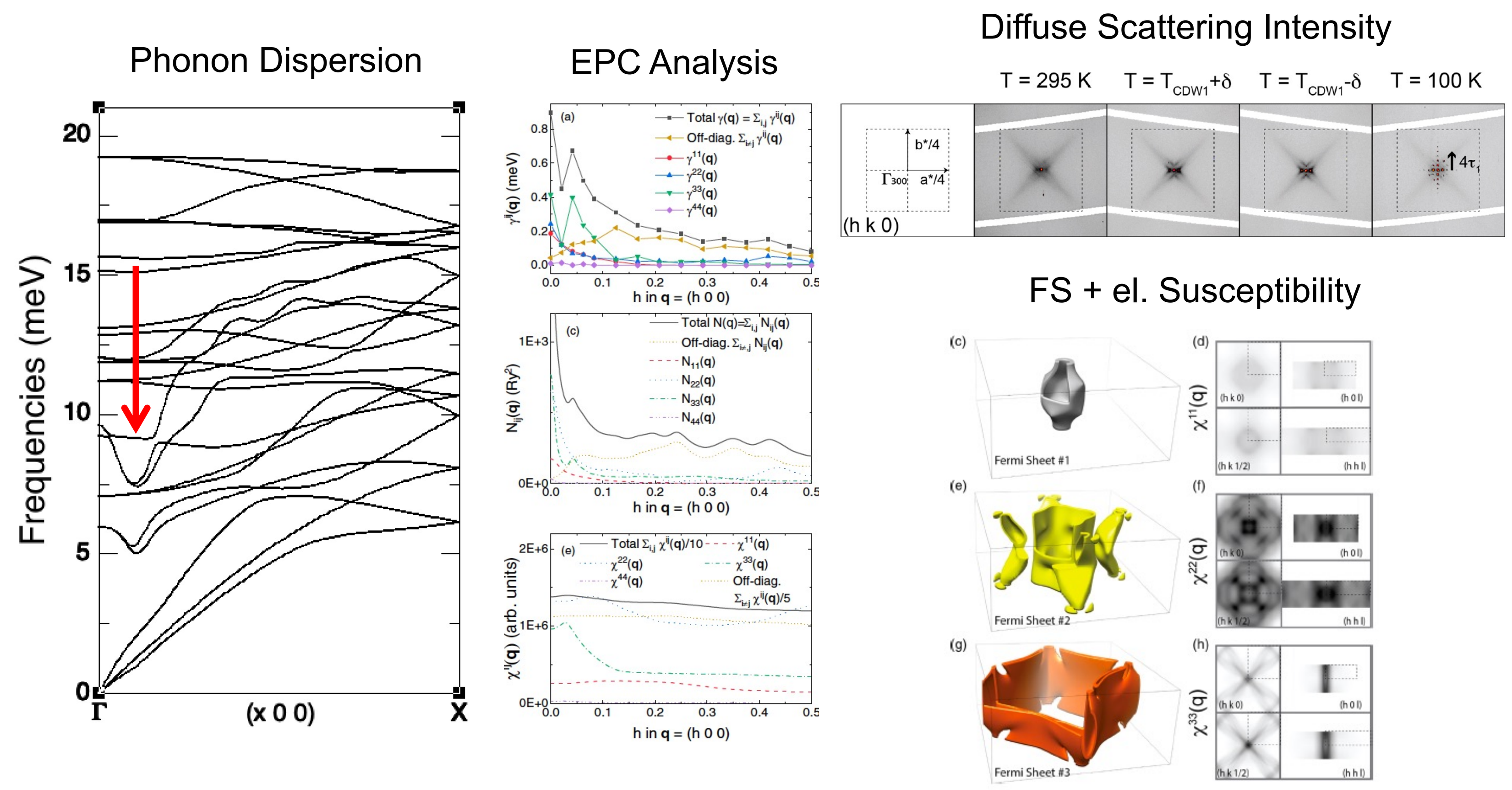
BaNi$_2$As$_2$ [5]: $T_{I\text{-}CDW}$=137 K, Q_c=(0.28,0,0)



- Soft mode: transverse vibration of Ni and As
- Near Q_c, slightly enhanced EPC matrix elements
- Doping/pressure: Complex phase diagram and CDW orders
- Ni-Ni bond ordering: local orbital fluctuations?

Dirac Semimetal

LaAgSb$_2$ [6]: $T_{CDW1/2}$ = 207 K/187 K; $Q_{c1/2}$=(0.026,0,0)/(0,0,0.16)



- Dirac semimetal, layered tetragonal structure
- Q_{c1} due to nesting in FS #3 in combination with enhanced EPC
- Parallel FS originate from Dirac-like points in band structure
- Diffuse scattering mimics intra-sheet susceptibility of FS #3

References

[1] B. Meyer *et al.*, MPI for Metal Research, Stuttgart
[2] R. Heid *et al.*, PRB **60**, R3709 (1999); PRB **81**, 174527 (2010)
[3] F. Weber *et al.*, PRL **107**, 107403 (2011); PRB **87**, 245111 (2013)
[4] F. Weber *et al.*, PRL **107**, 266401 (2011); M. Maschek et al., PRB **94**, 214507 (2016)
[5] A.R. Pokharel *et al.*, Commun. Phys. **5**, 141 (2022); S.M. Souliou *et al.*, PRL **129**, 247602 (2022); C. Meingast *et al.*, PRB **106**, 144507 (2022)
[6] A. Bosak *et al.*, PR Research **3**, 033020 (2021)

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