Low-Thermal Conductivity in Layered vdW Antiferromagnet $GdTe_3$: A Charge Density Wave Material

Prabir Dutta, Sushmita Chandra, Koyendrila Debnath, Umesh V. Waghmare and Kanishka Biswas

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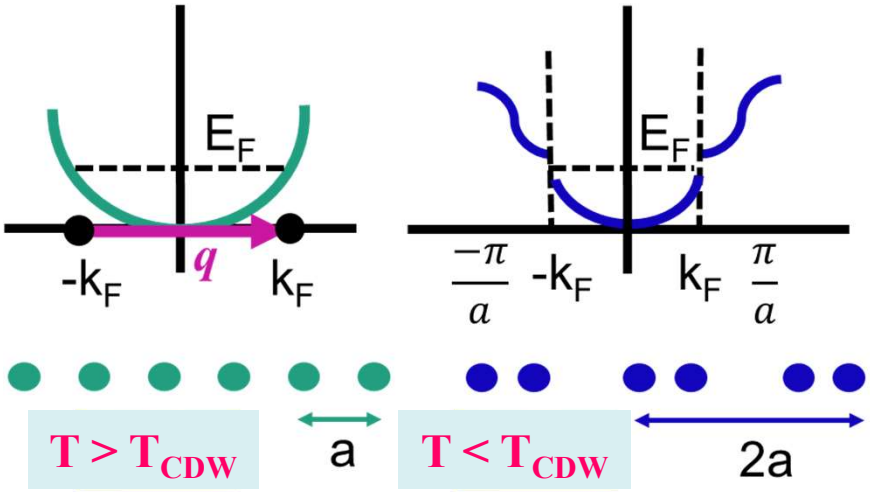
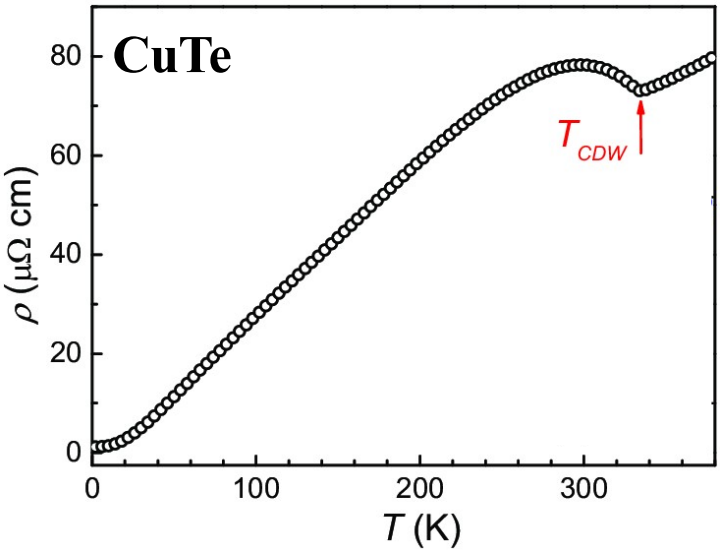
JNCASR

What is Charge Density Wave (CDW)?

Peierls distortion: 1D metal chain ***unstable***



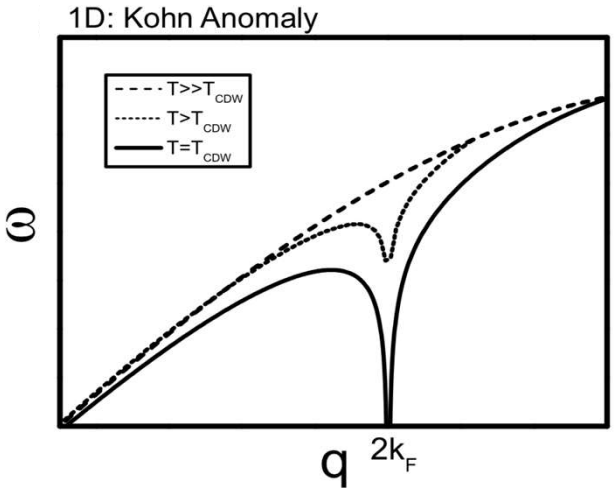


Peierls Distortion

Metal to Insulator

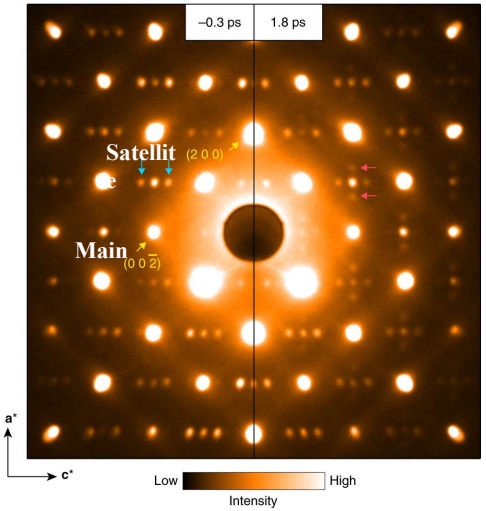
Band splitting at Fermi surface nesting vector, $q = 2k_F$

CDW **is a** ***static modulation*** **of** ***conduction electrons*** **and is a Fermi-surface driven phenomenon usually accompanied by a periodic distortion of the lattice.**



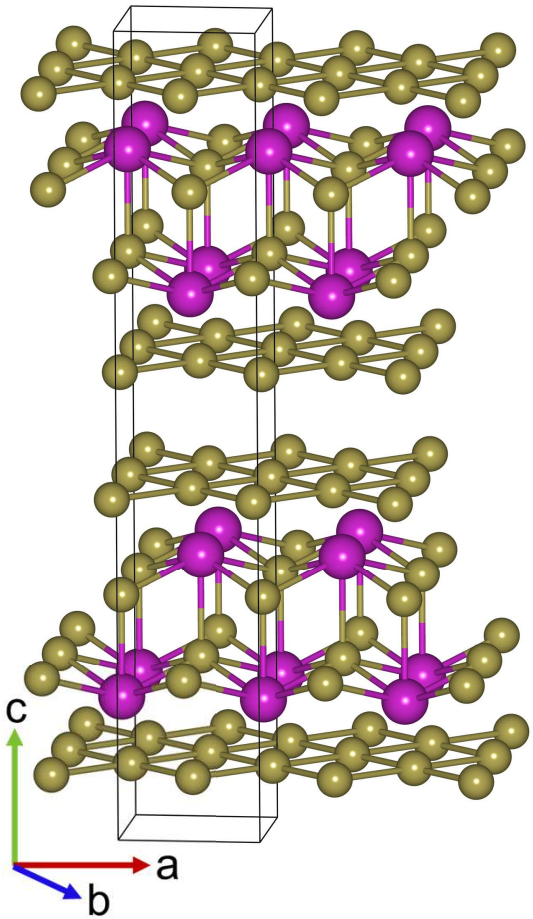
Kohn anomaly in acoustic phonon branch

Superlattice spots **in Electron Diffraction ($LaTe_3$)**



Peierls R. E., **1955**, Quantum Theory of Solids (Oxford Univ Press, New York)

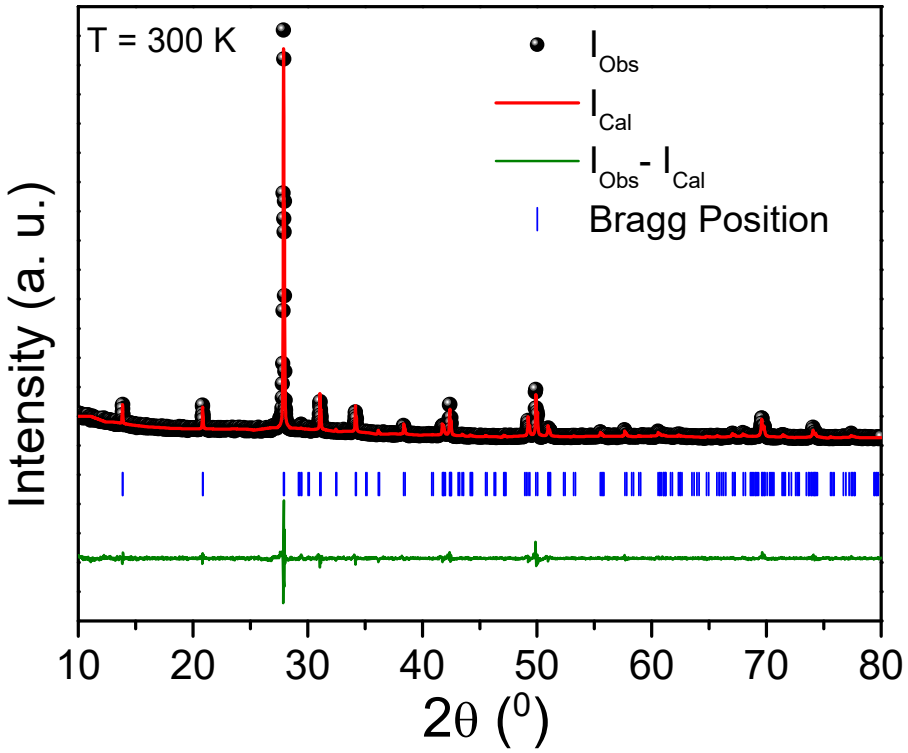
$GdTe_3$: A Quasi 2D vdW Antiferromagnet

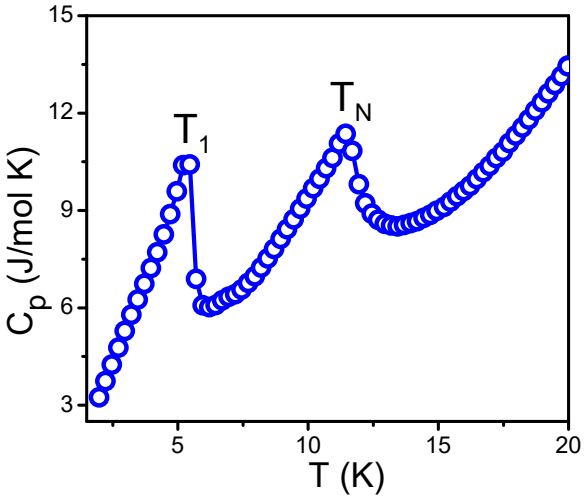


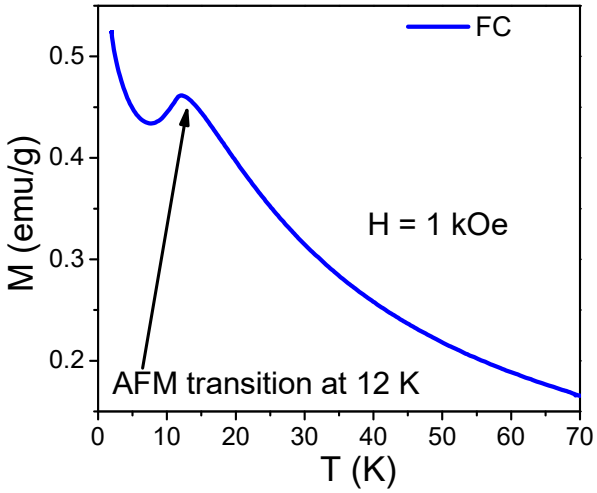
Gd Te

Space Group: ***Cmcm***

- ***Layers*** are stacked along c-axis (perpendicular to **Te sheets**)
- **Square planar Te sheets**
- **GdTe corrugated slabs**

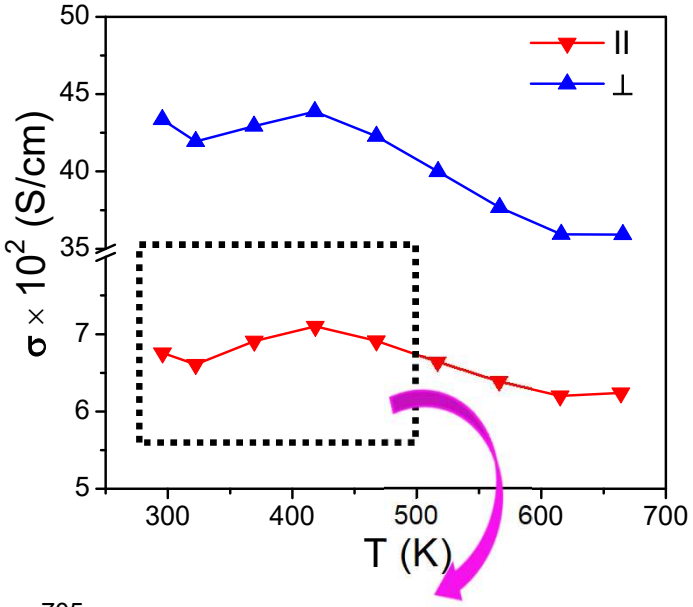


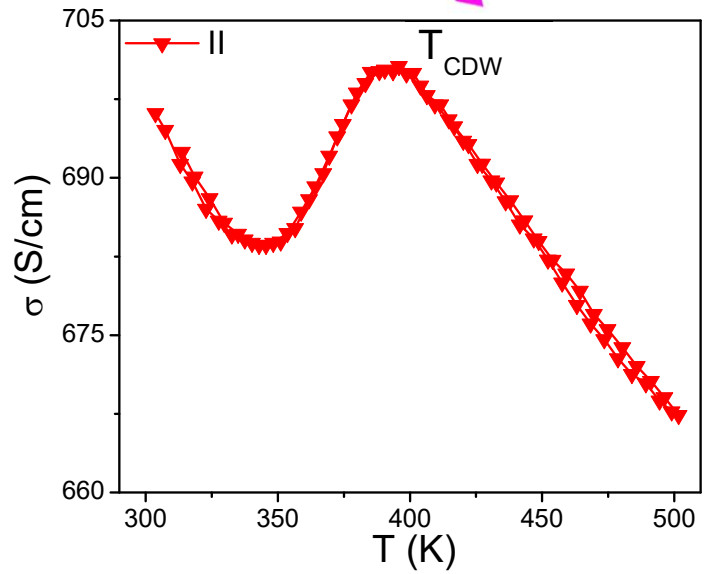




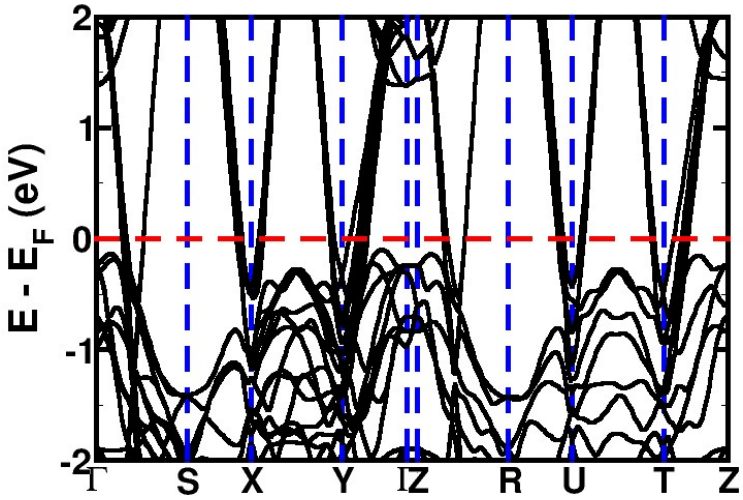
Square-net arrangement of Te ***unstable***: **origin of CDW**

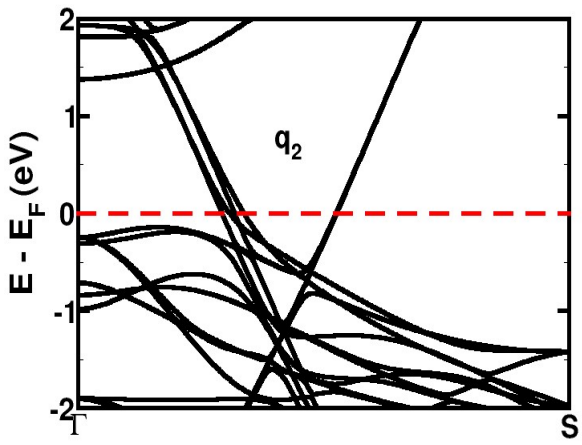
Electrical Conductivity and Electronic Structure of $GdTe_3$

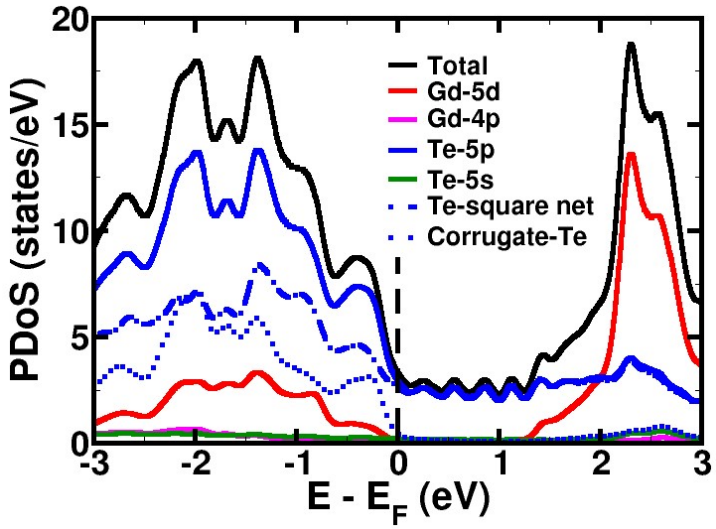




Electronic Structure & PDOS (without SOC)







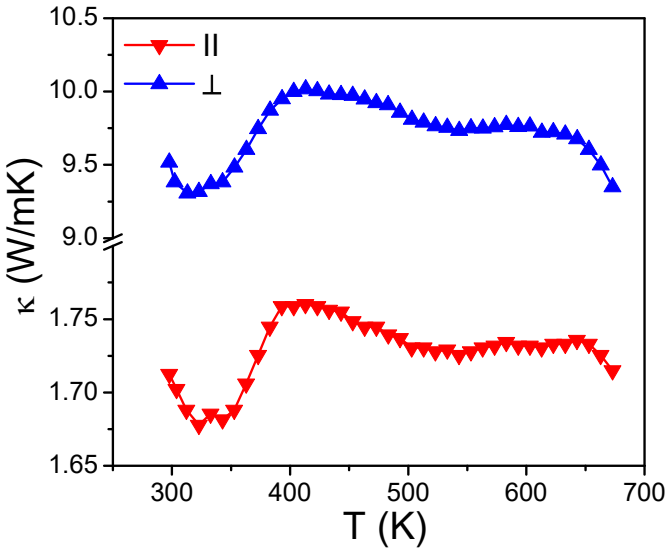
$$\mu = \frac{q}{m*}\tau$$

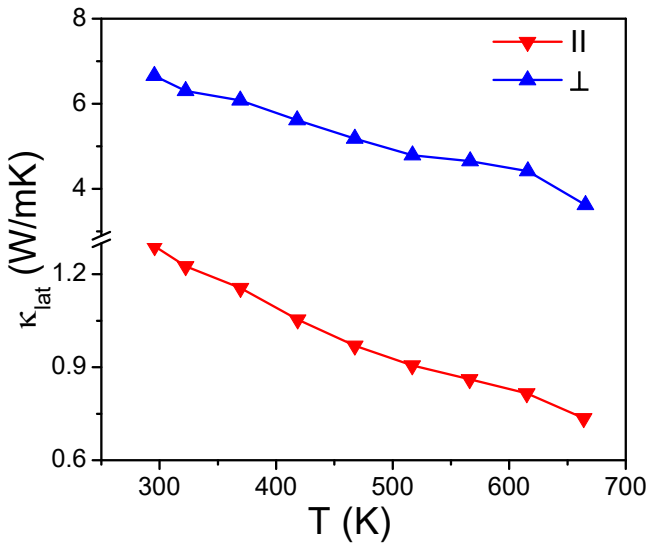
Nesting vector (q_2) in electronic structure

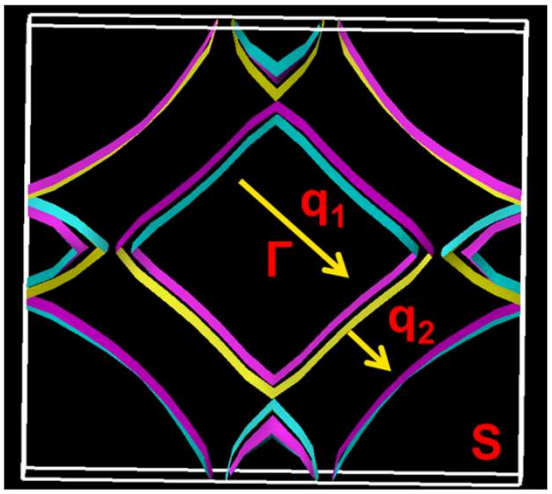
- Steep linearly dispersive bands giving rise to high mobility
- Contribution of *p*-orbitals of Te bilayer significant at E_F

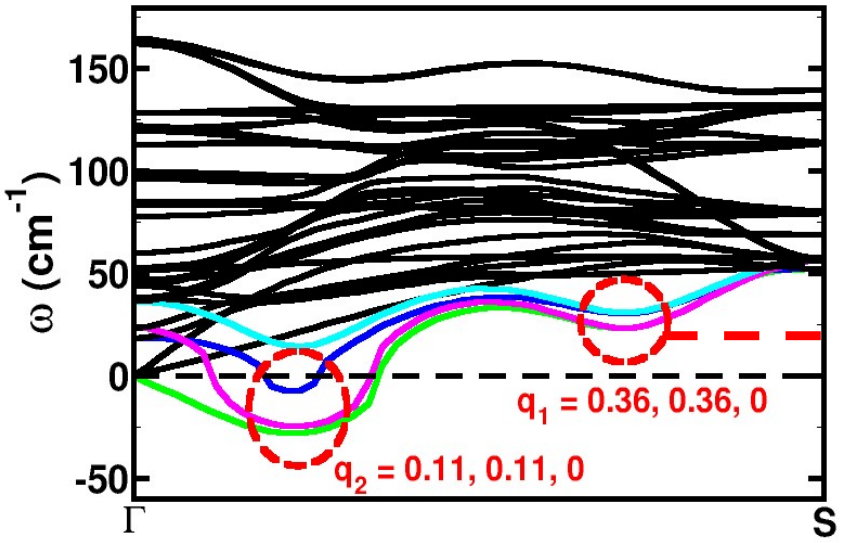
In collaboration with Prof. Waghmare's group

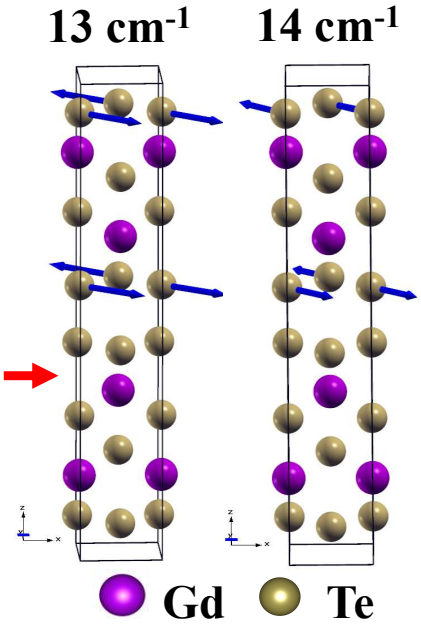
Thermal Conductivity Associated with CDW Instability











Strong Fermi Surface Nesting along Γ-S :

Many electronic states on the Fermi surface can be **scattered by a phonon with nesting wave vector** to other states on the Fermi-surface

Instability at q_2 and softening at q_1 (along **Γ-S**)

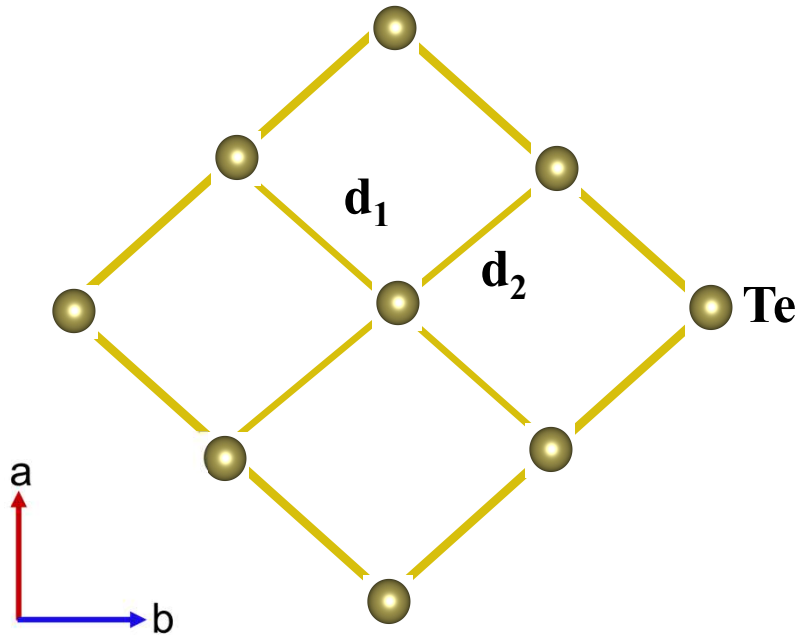
Kohn anomaly at q_1, induced by **displacements of Te atoms** in **square-net sheets**

Conclusions

$T_{CDW} \sim 380$ K

- CDW phase
- *Distorted*
- *Insulator; stable*

- Non CDW
- *Undistorted*
- *Metallic; unstable*



Distorted Te square sheets ($d_1 \neq d_2$)

- **Soft optical phonons scatters heat carrying phonons giving rise to low thermal conductivity κ**
- **Bulk low-dimensional layered materials with *CDW instability* are promising candidates for new thermoelectric materials**

Acknowledgements

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Thank You