ICN2 Institut Català de Nanociència i Nanotecnologia

EXCELENCIA SEVERO OCHOA

Charge Density Waves in 2D Materials

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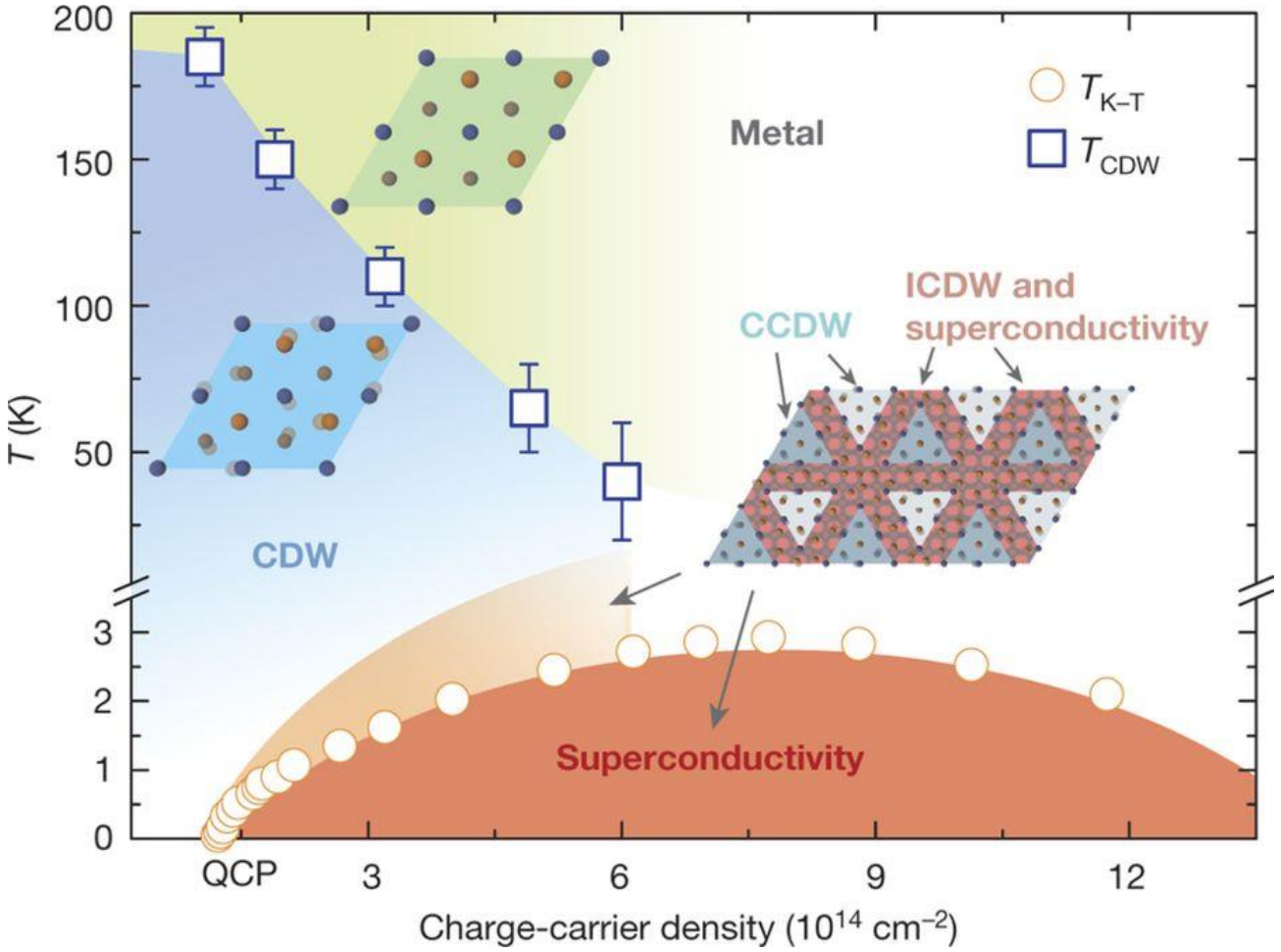
Motivation

$1T-TiSe_2$

Nature **529**, 185–189 (14 January 2016)



Contents

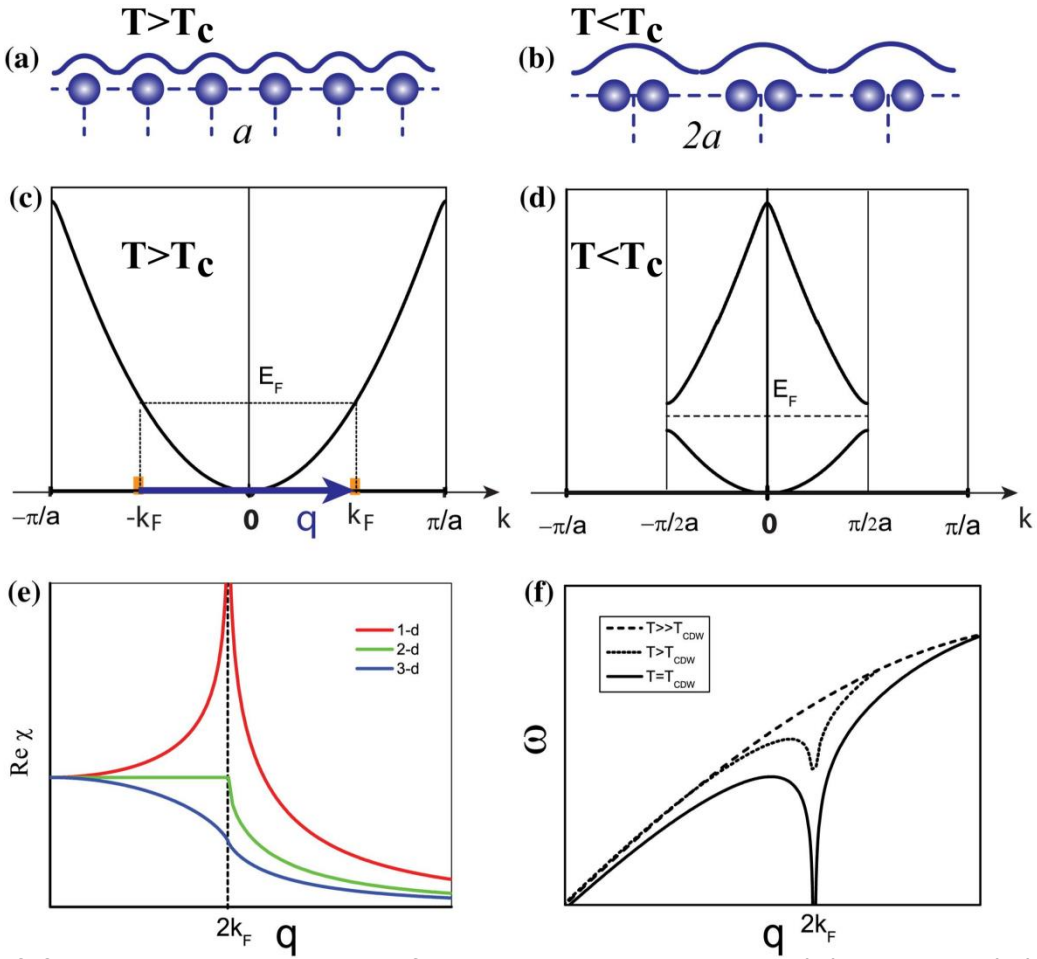
→ What is a charge density wave?

→ Electronic structure of TiSe2

→ Phonons' role and the 2x2 CDW phase

→ Doping effect on the CDW phase

What is a Charge Density Wave?

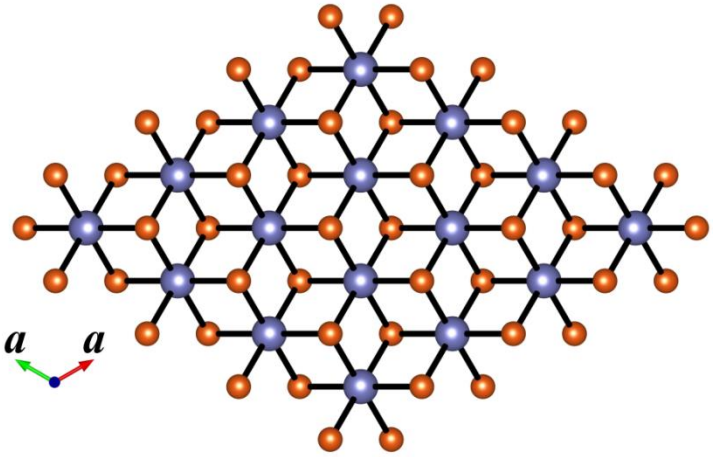


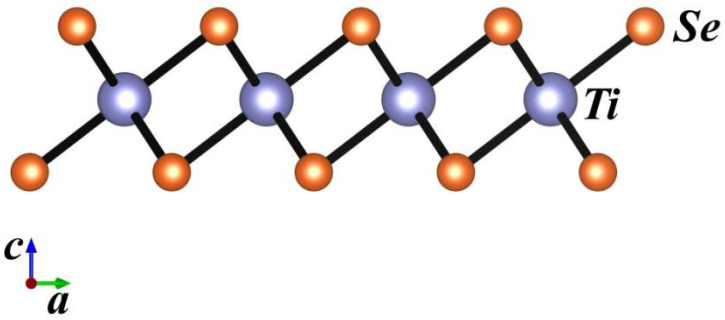
- Half-filled electron band of the 1D atomic above (c), below (d) Tc
- Real part of the Lindhard function for 1D, 2D and 3D free electron gas (e)
- Phonon dispersion of 1D atomic chain at different temperatures (f)

Adv. Phys. X 2 3 622-640 (2017)

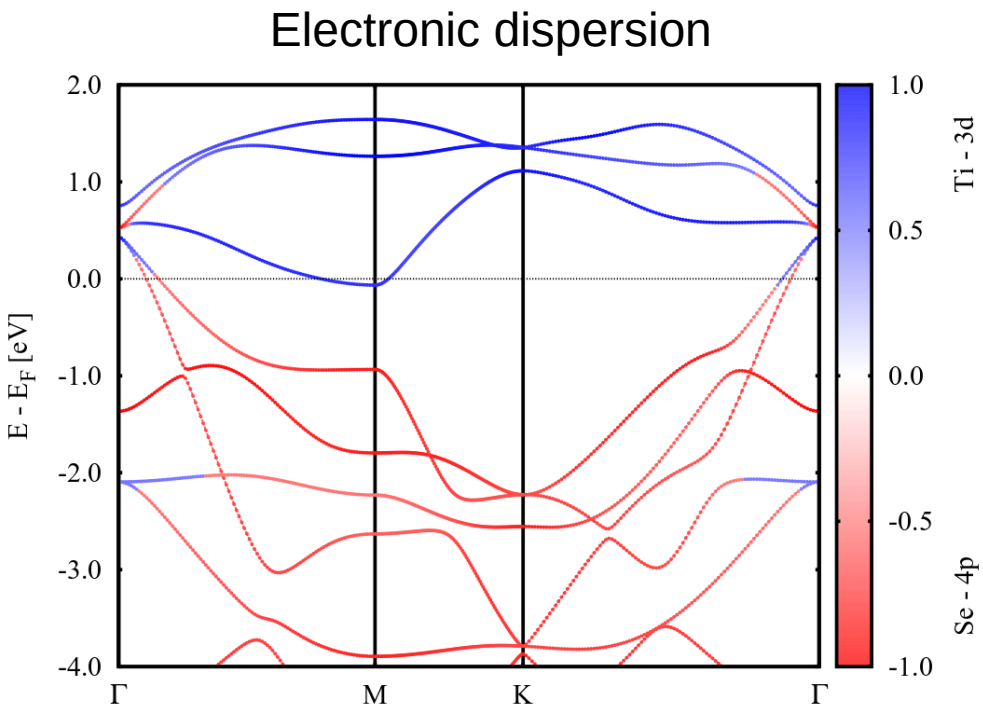
TiSe2 – Intro

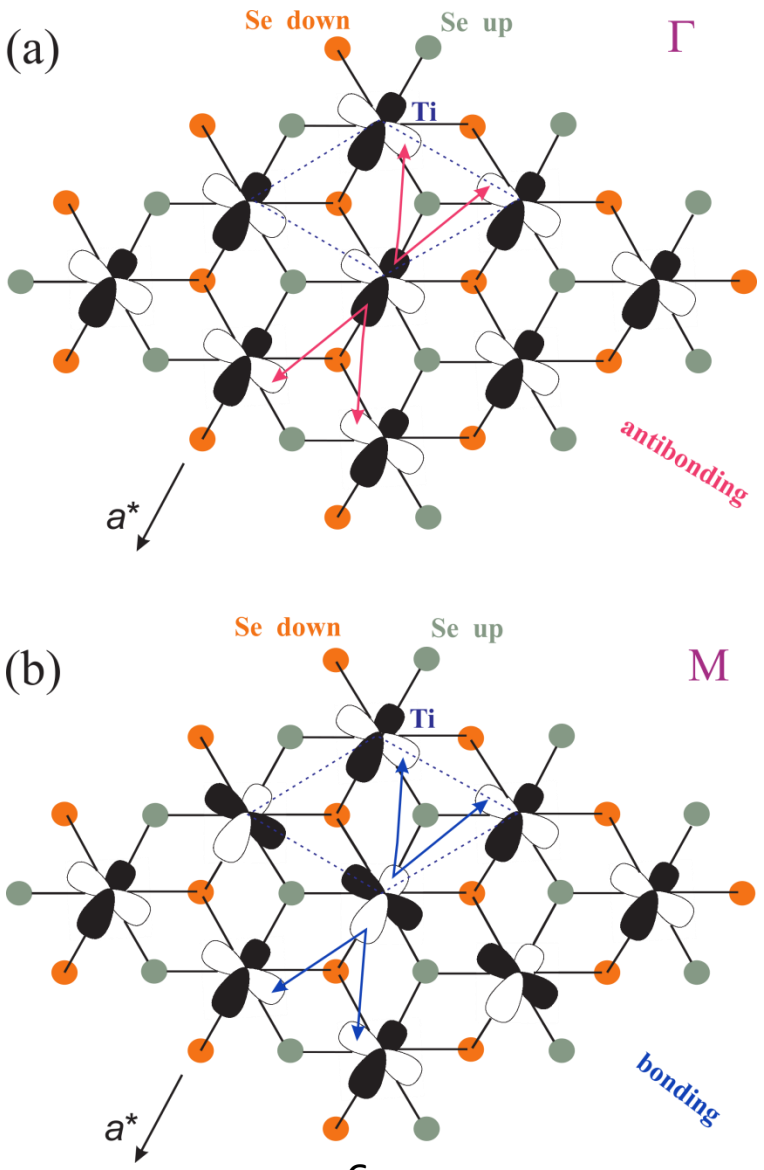
- Semi-metallic (d^0)
- Phase transition at ~230 K
- 2x2 CDW modulated structure
- Opens gap at Fermi level
- Commensurate → Incommensurate with doping





TiSe2 – Semi-metallic character





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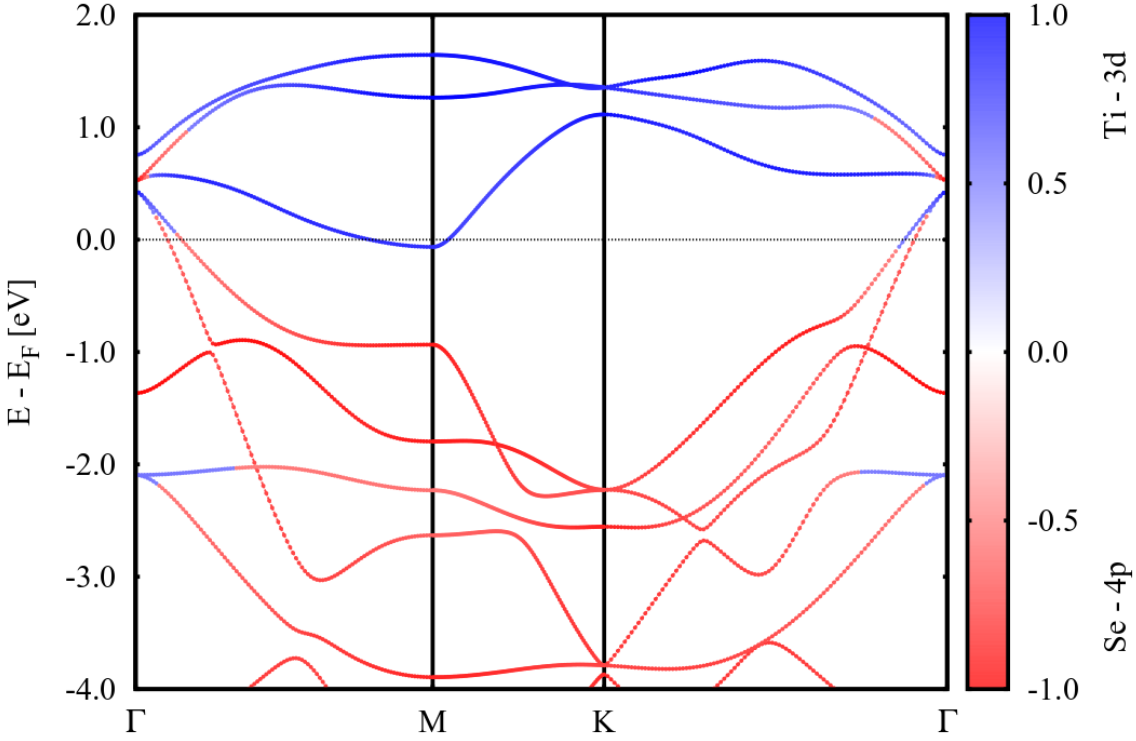
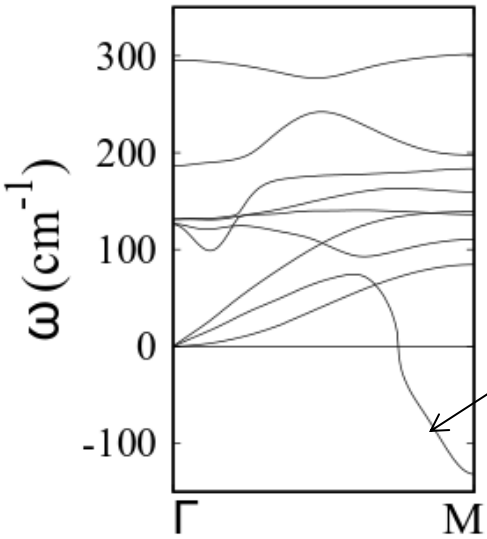
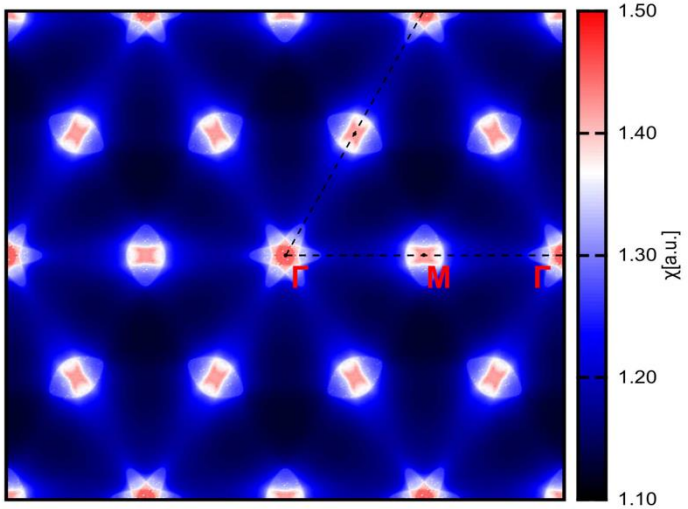
TiSe2 – Electrons and Phonons

Electronic dispersion



Phononic dispersion





Lindhard function mapping

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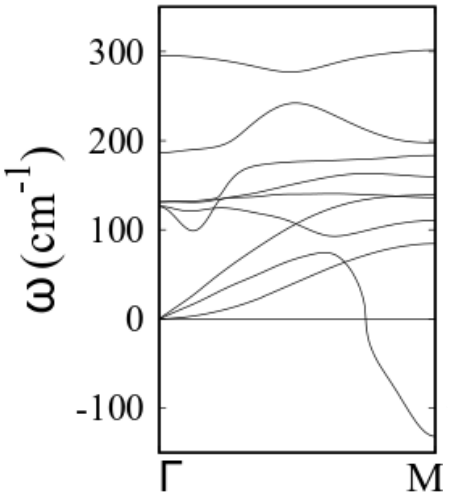
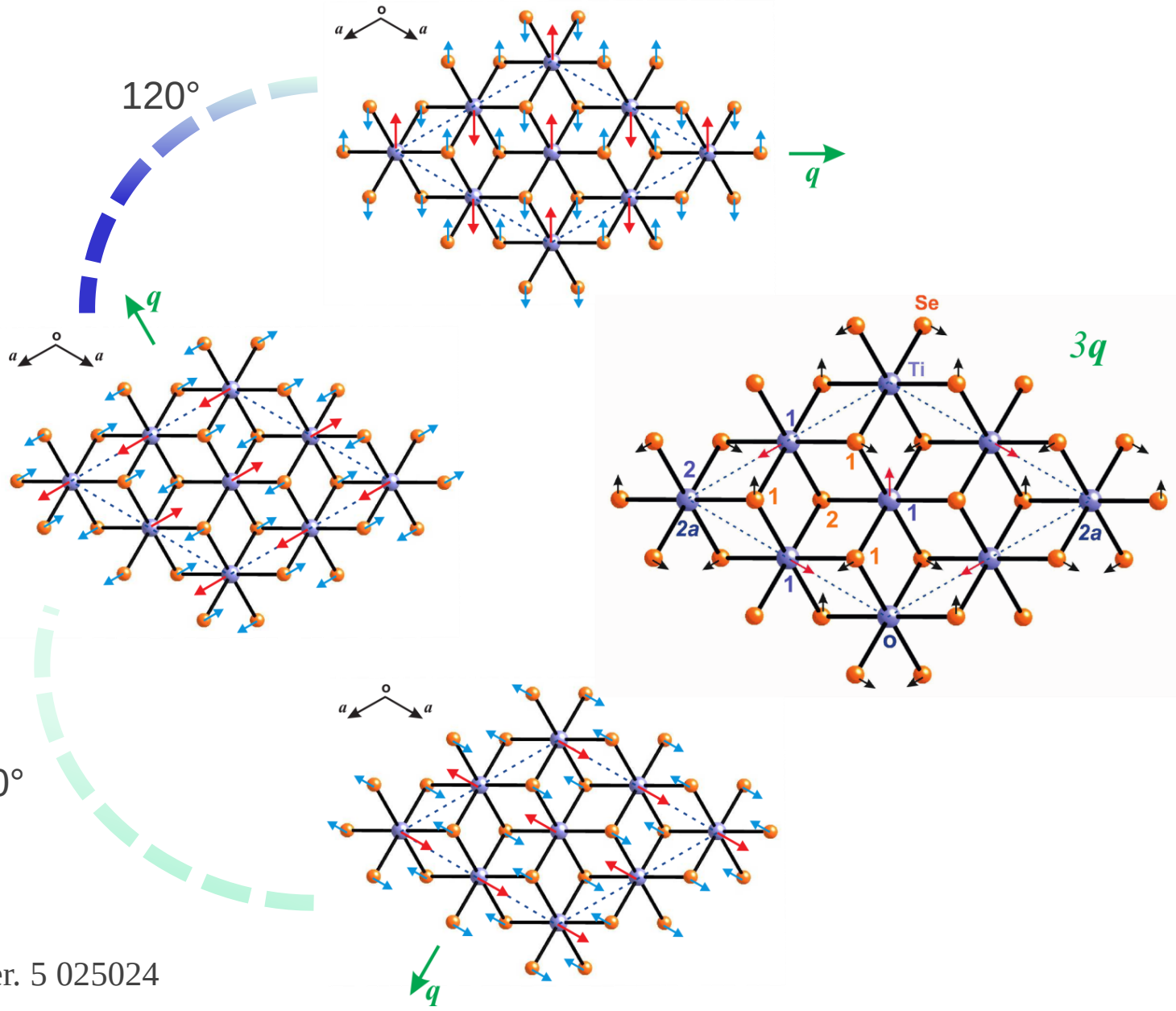
TiSe2 – Phonons Behaviour





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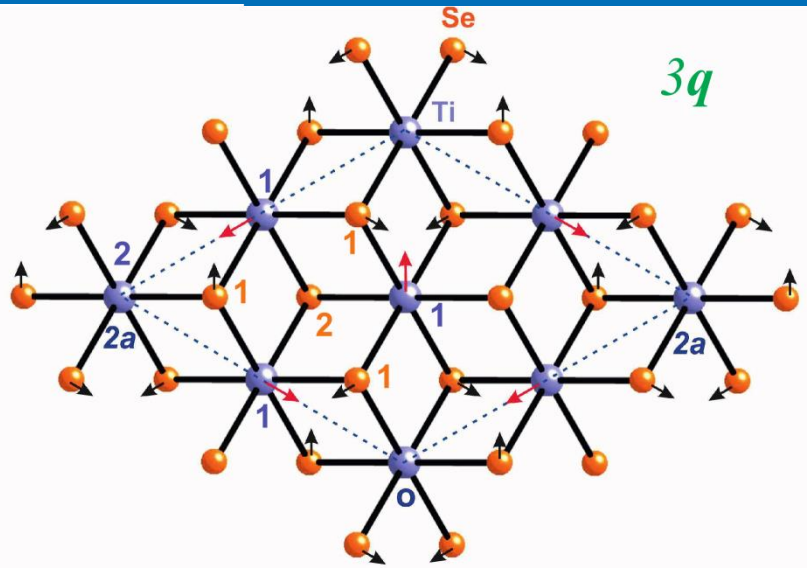
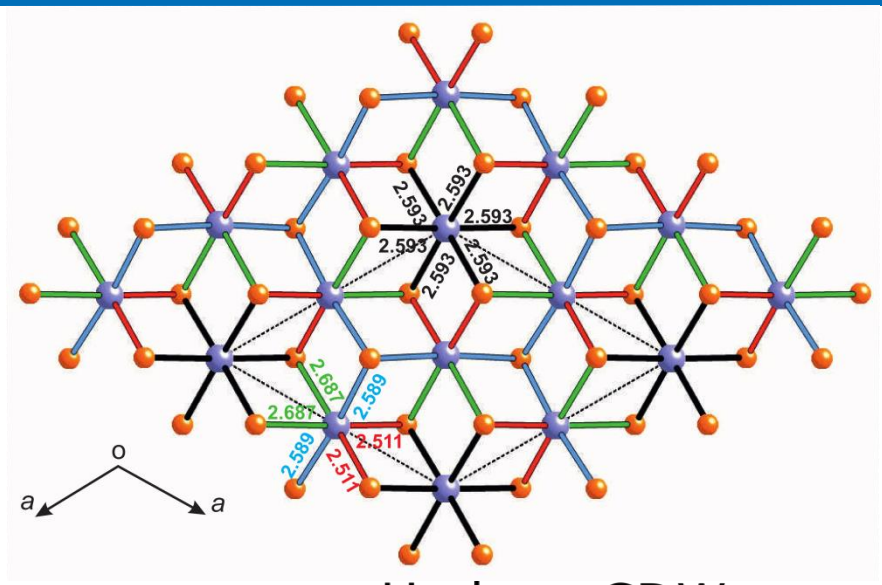
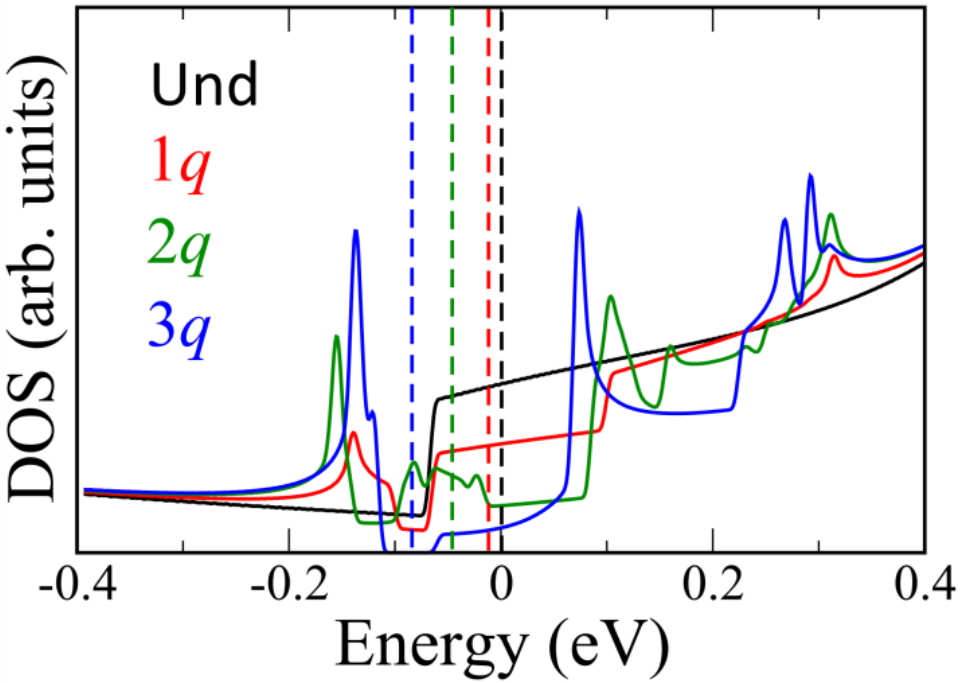
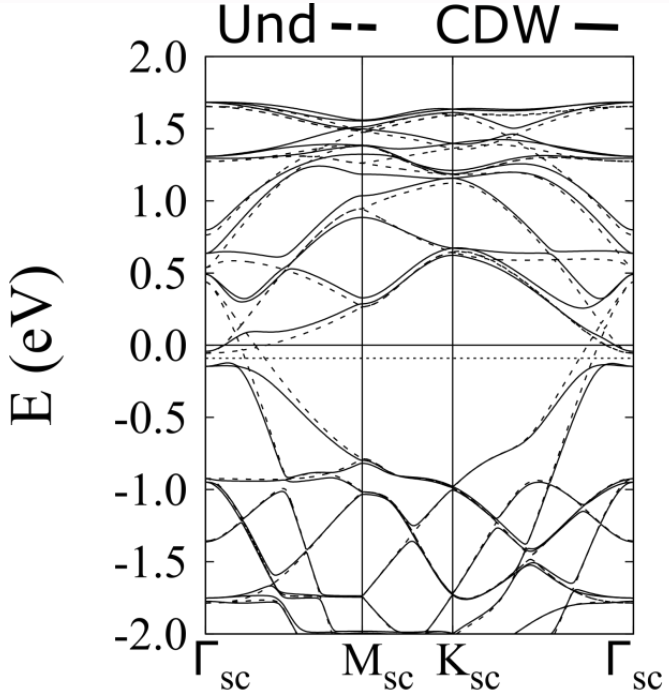
TiSe2 – 2x2 CDW phase

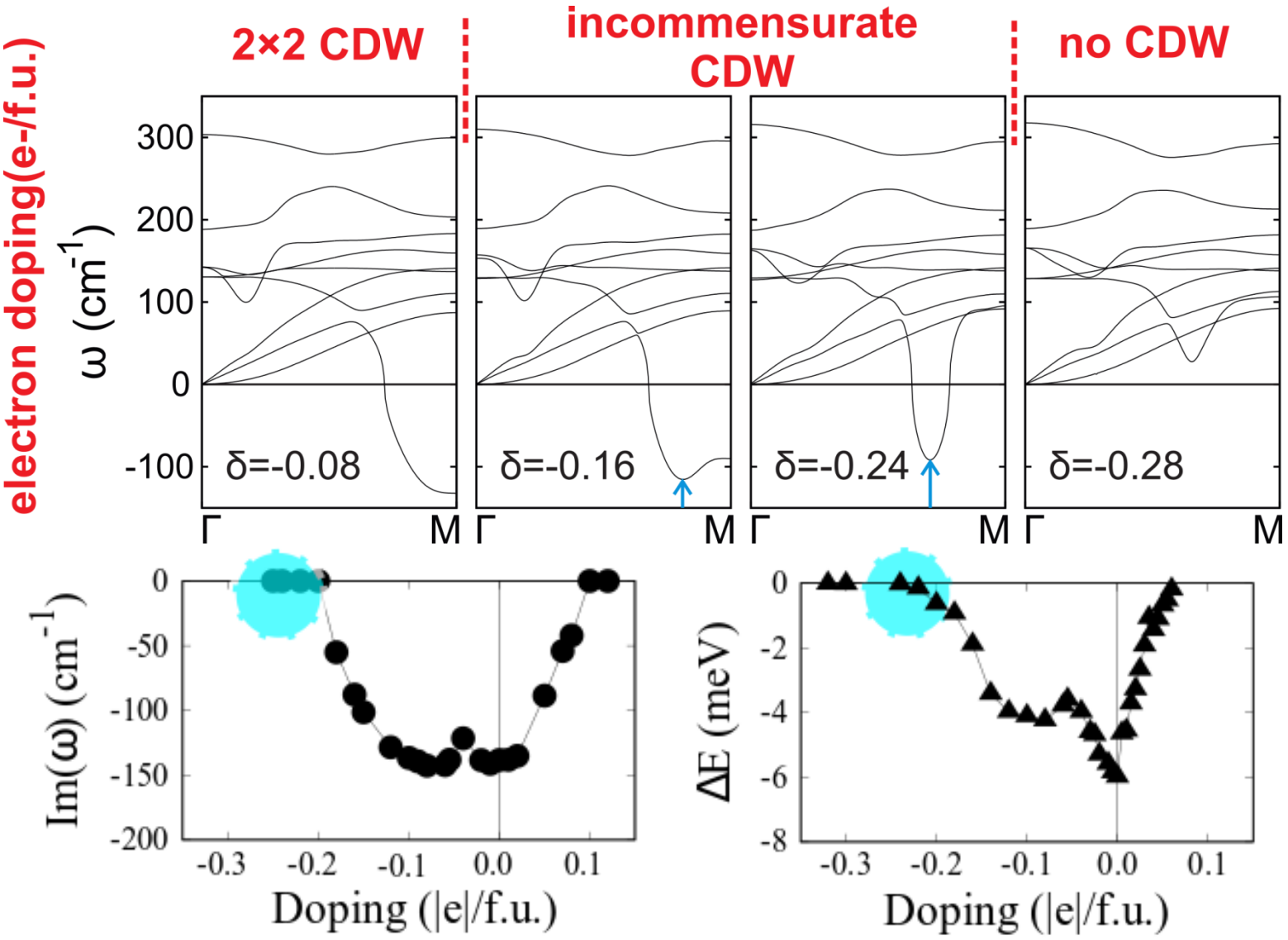








TiSe2 – Doping effect



Conclusion

- Electronic structure character
- Phonon instability at M
- 1Q phonon condensation → 2x1 CDW
- 3Q phonon condensation → 2x2 CDW
- Doping → Incommensurate CDW
- Similar mechanism in single-layer $TiTe_2$