Interaction of graphene with metallic and semiconductor surfaces
An ab initio approach

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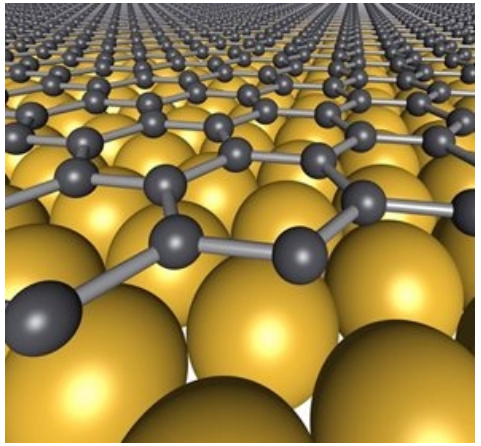
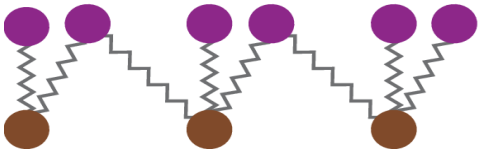
Interaction graphene/substrate



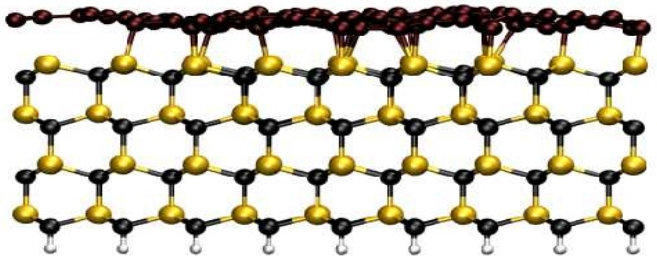
The physical properties of graphene depends critically on the environment



Change in phonon modes allows to characterize graphene/substrate interaction

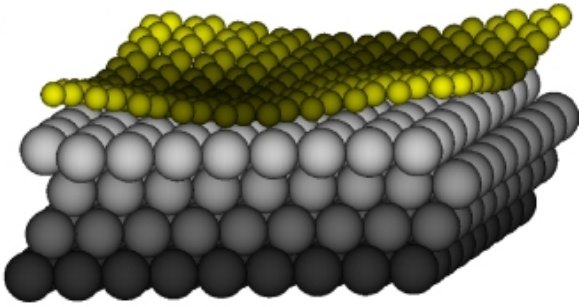
Ab-initio calculations of the lattice dynamics

silicon carbide



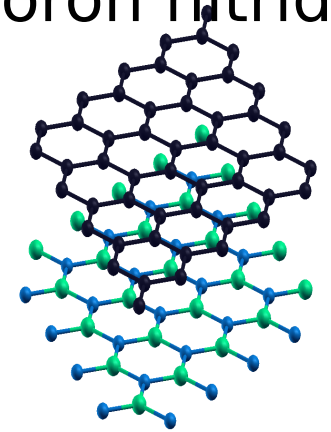
Phys. Rev. B82, 121416R (2010)

iridium



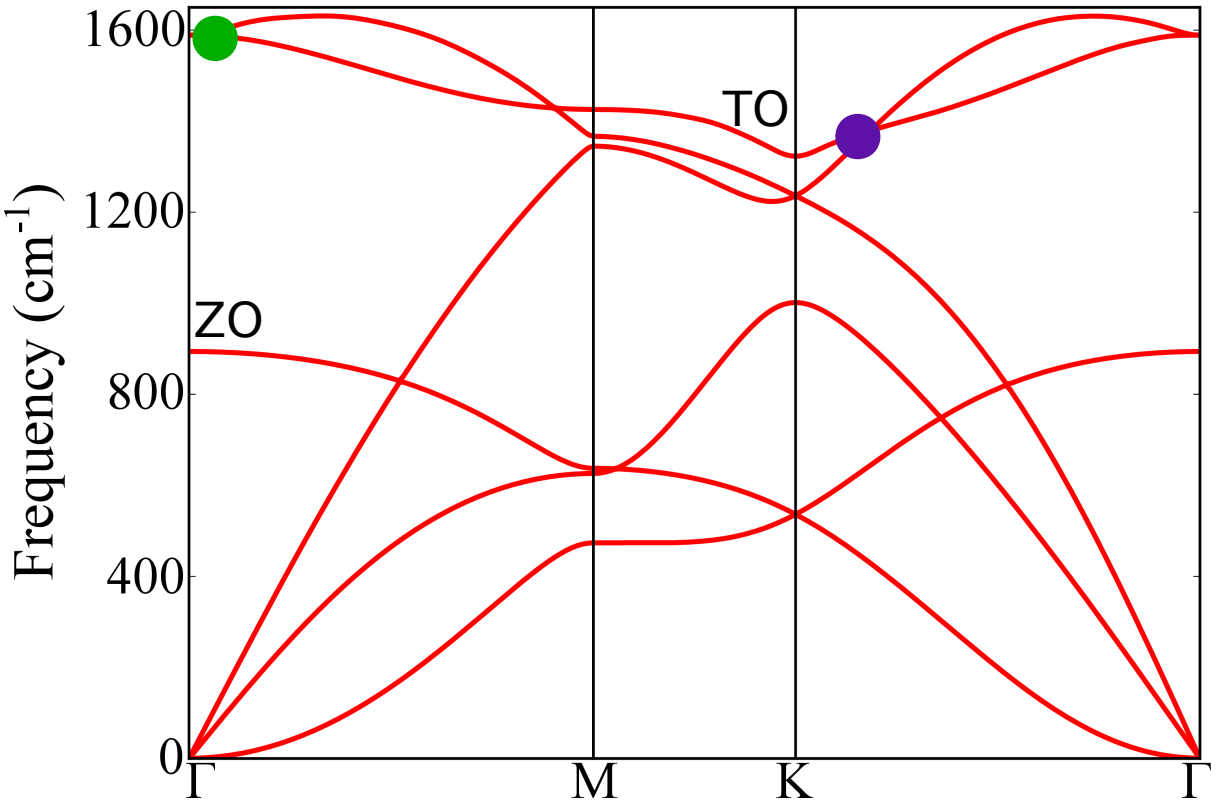
J. Phys.: Condens. Matter **24** 424215 (2012)

boron nitride



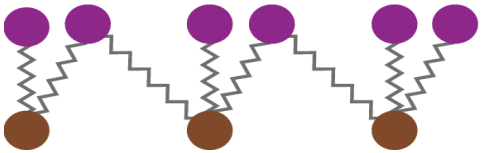
Comparison with Raman and electron energy loss spectroscopies

Graphene. Phonons



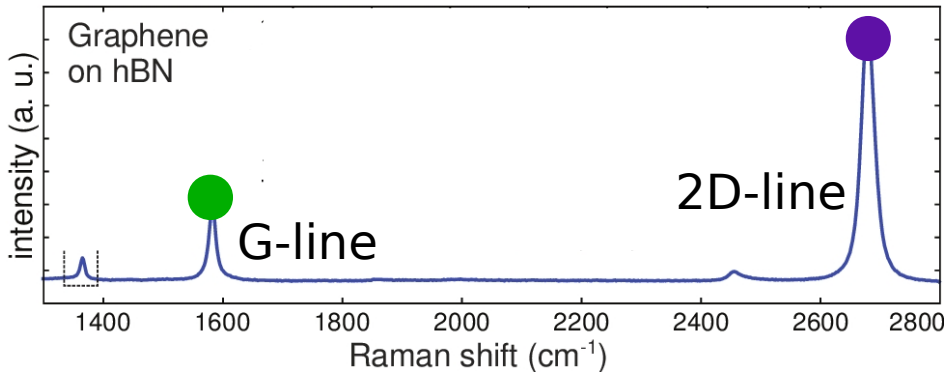
DFT-LDA gives good results for phonons...

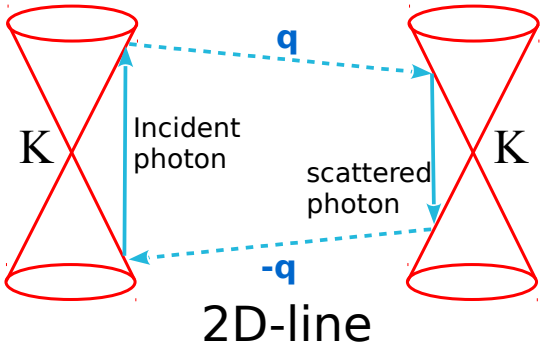
ZO phonon quantify the attachment of graphene to the substrate



... LDA fails to describe TO phonon at K-point (Kohn anomaly). GW approx.

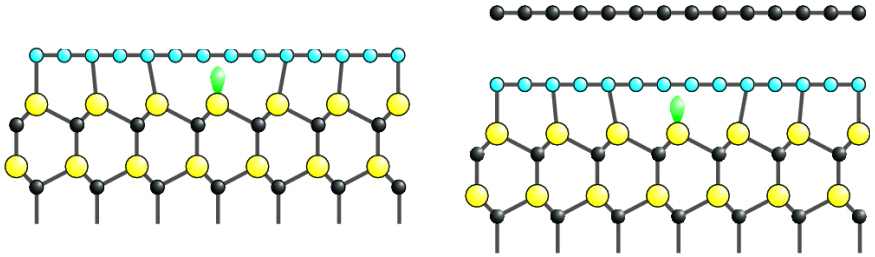
F Forster, AMS et. al. Phys. Rev. B 88, 085419 (2013)





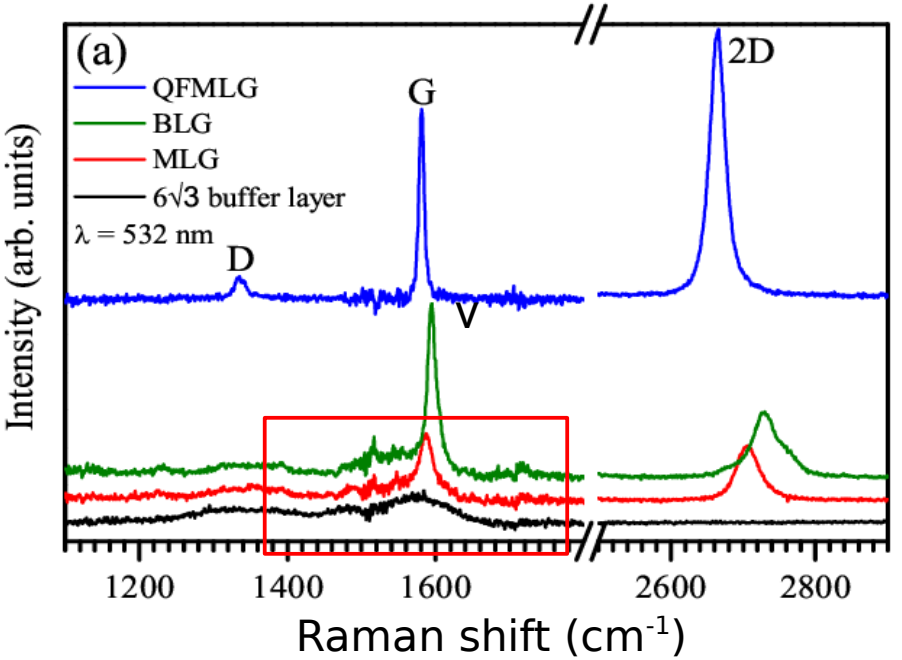
Graphene@SiC. Buffer layer

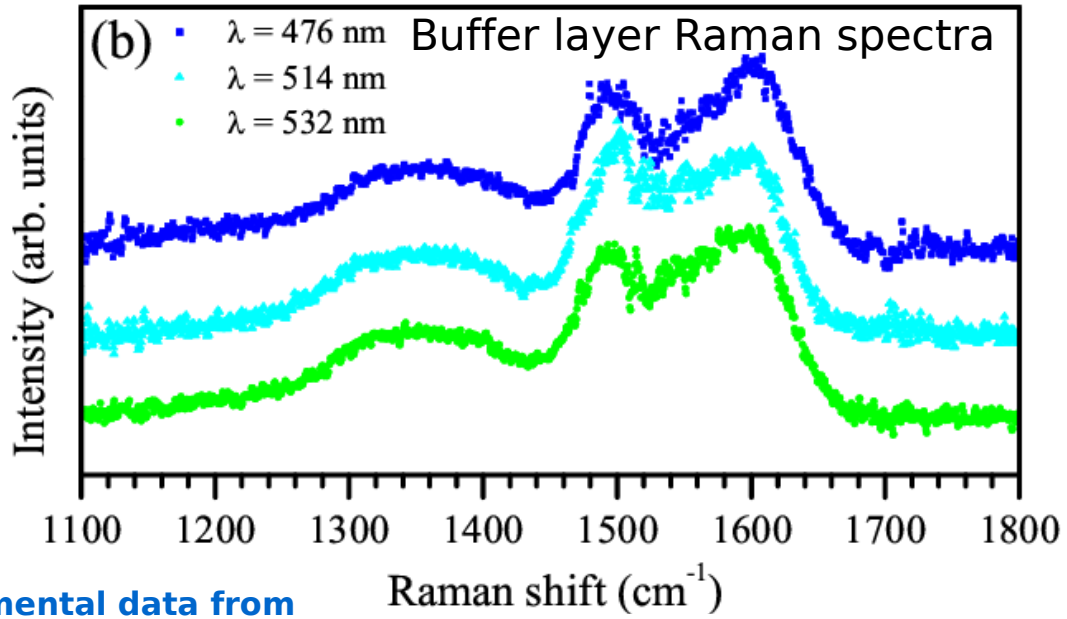
Buffer layer Epitaxial graphene



Hybridization π-states and SiC states.

Contribution of the buffer layer to the Raman spectrum of epitaxial graphene on SiC?





Spectra are not compose of discrete peaks.

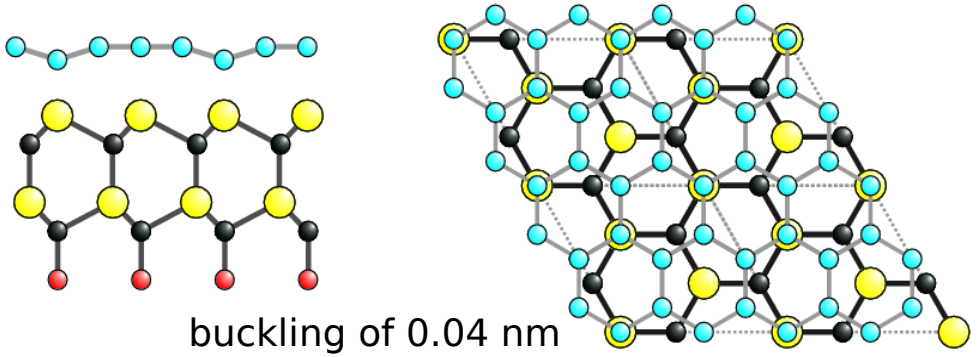
Resemble a density of states?

Experimental data from F Fromm & T. Seyller

F Fromm, MH Oliveira Jr, AMS et. al., New Journal of Physics, 15 043031 (2013)

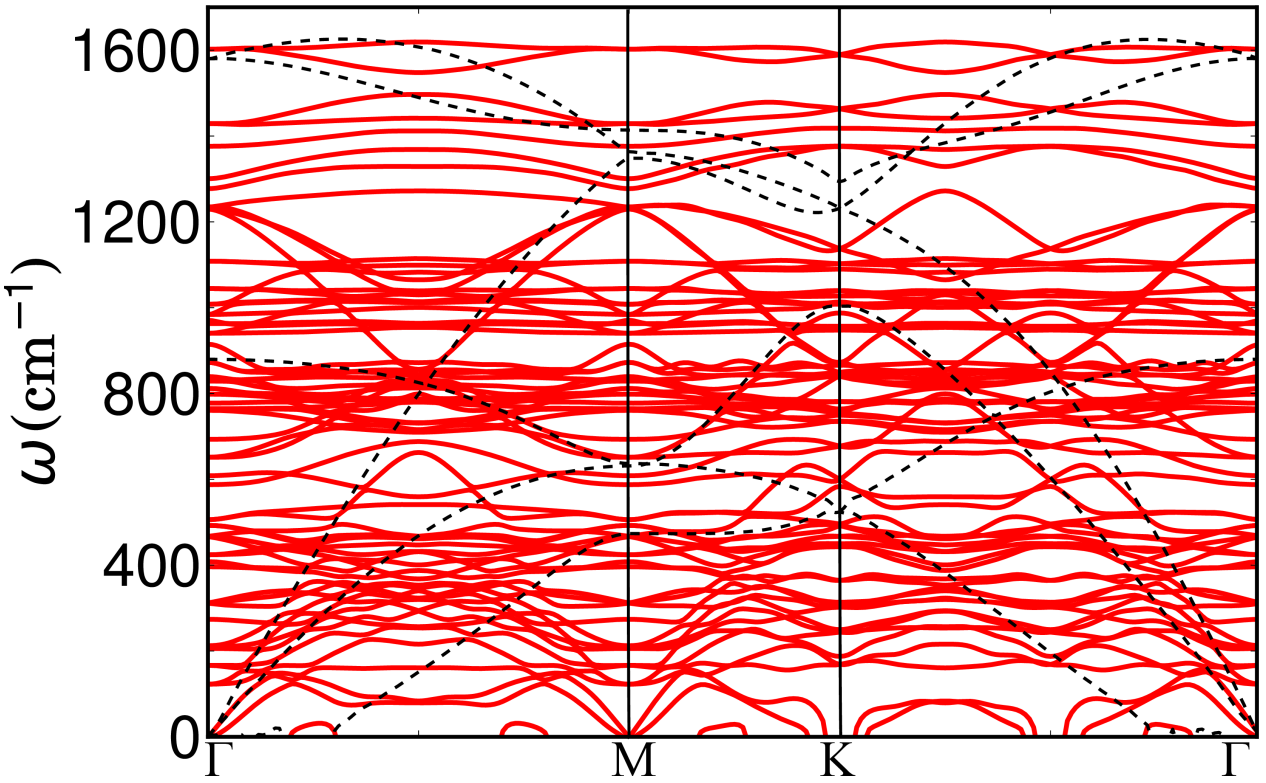
Graphene@SiC. Buffer layer

Calculations in a 2x2 graphene unit cell.



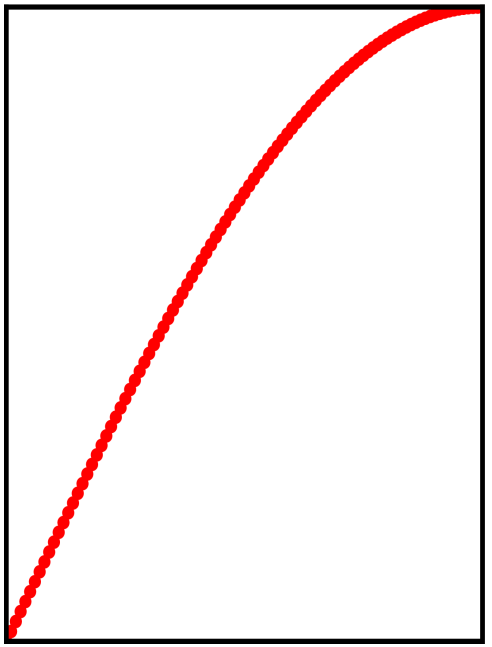
buckling of 0.04 nm

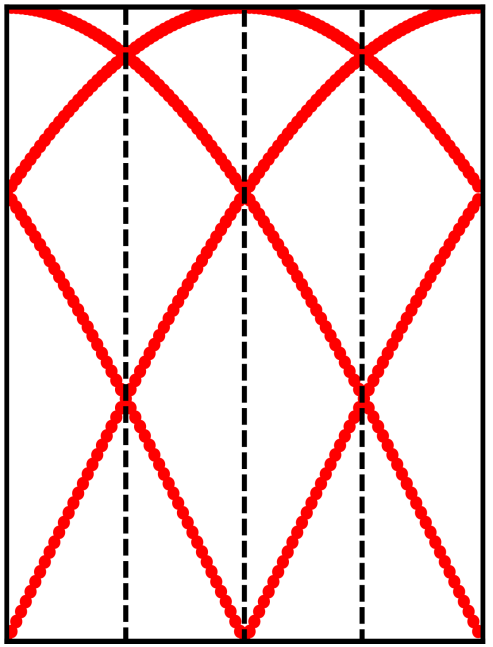
- Calculations in large supercells fold the phonon dispersion relation.
- Unfolding of the phonon modes for easier interpretation of our results.

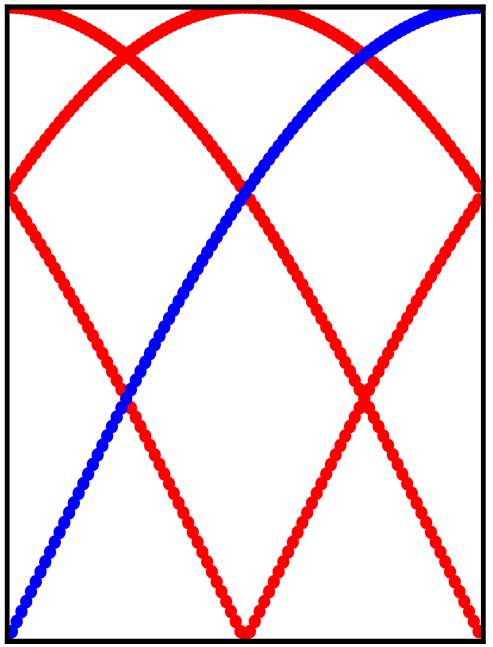


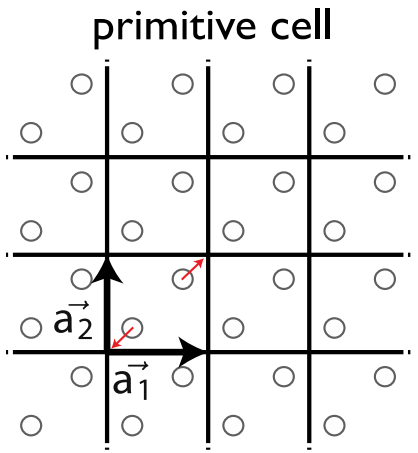
F Fromm, MH Oliveira Jr, AMS et. al.,
New Journal of Physics, 15 043031 (2013)

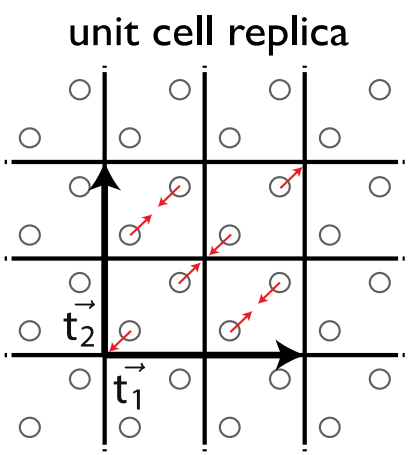
Graphene@SiC. un-folding

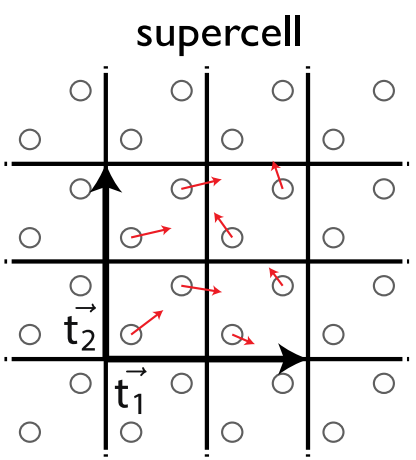




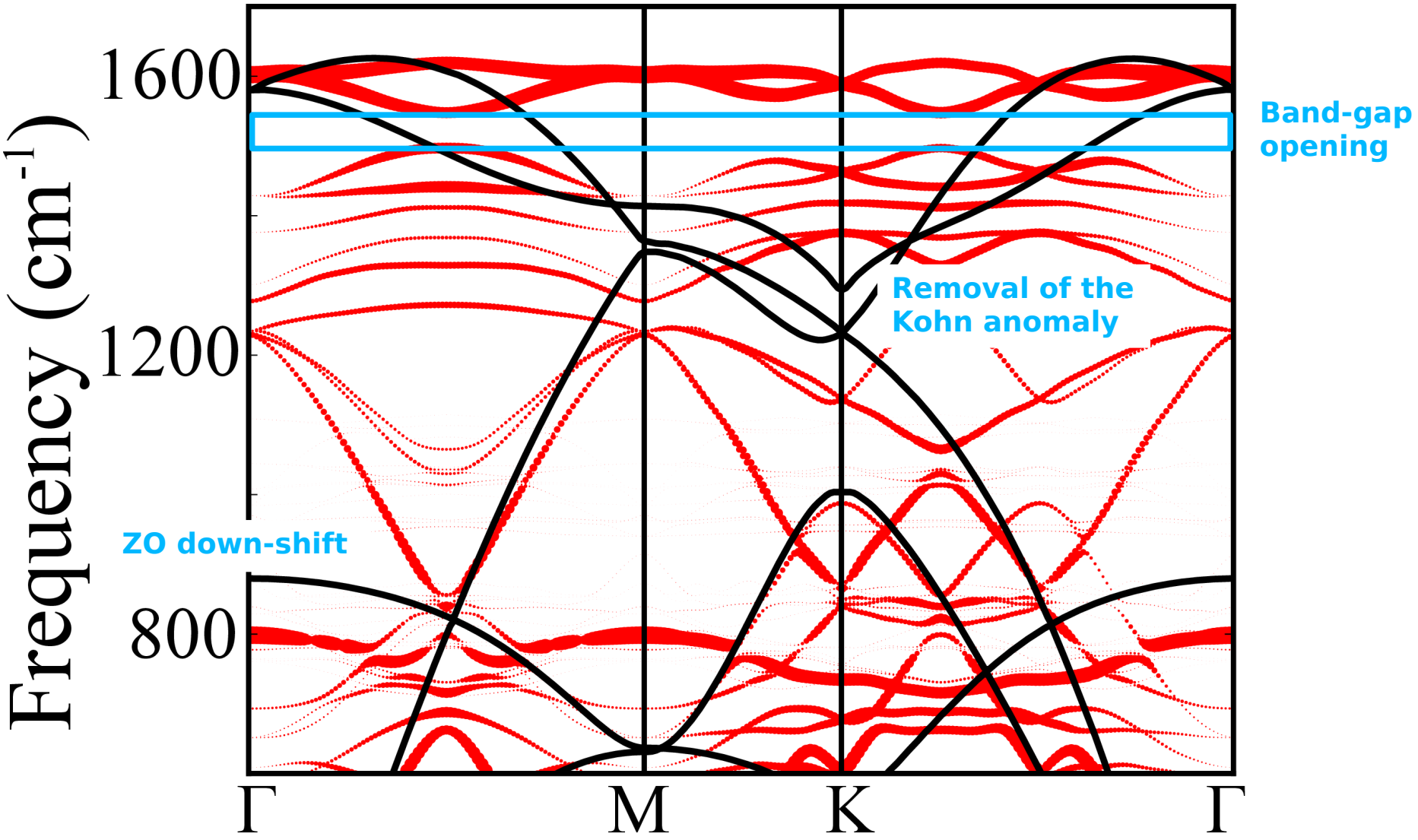






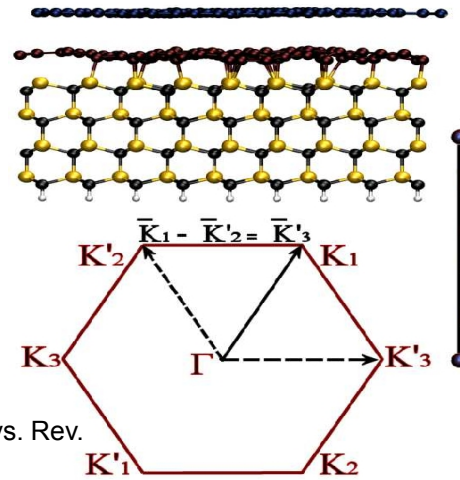


Graphene@SiC. Buffer layer

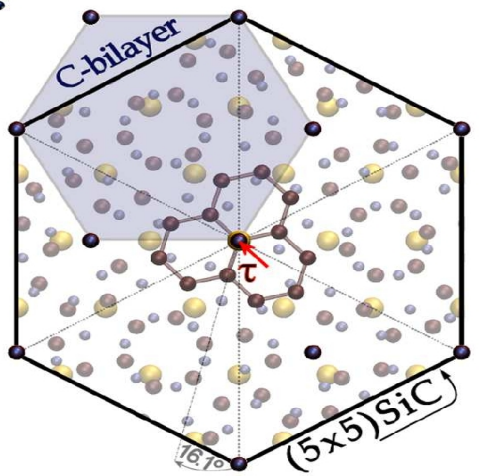


F Fromm, MH Oliveira Jr, AMS et. al.,
New Journal of Physics, 15 043031 (2013)

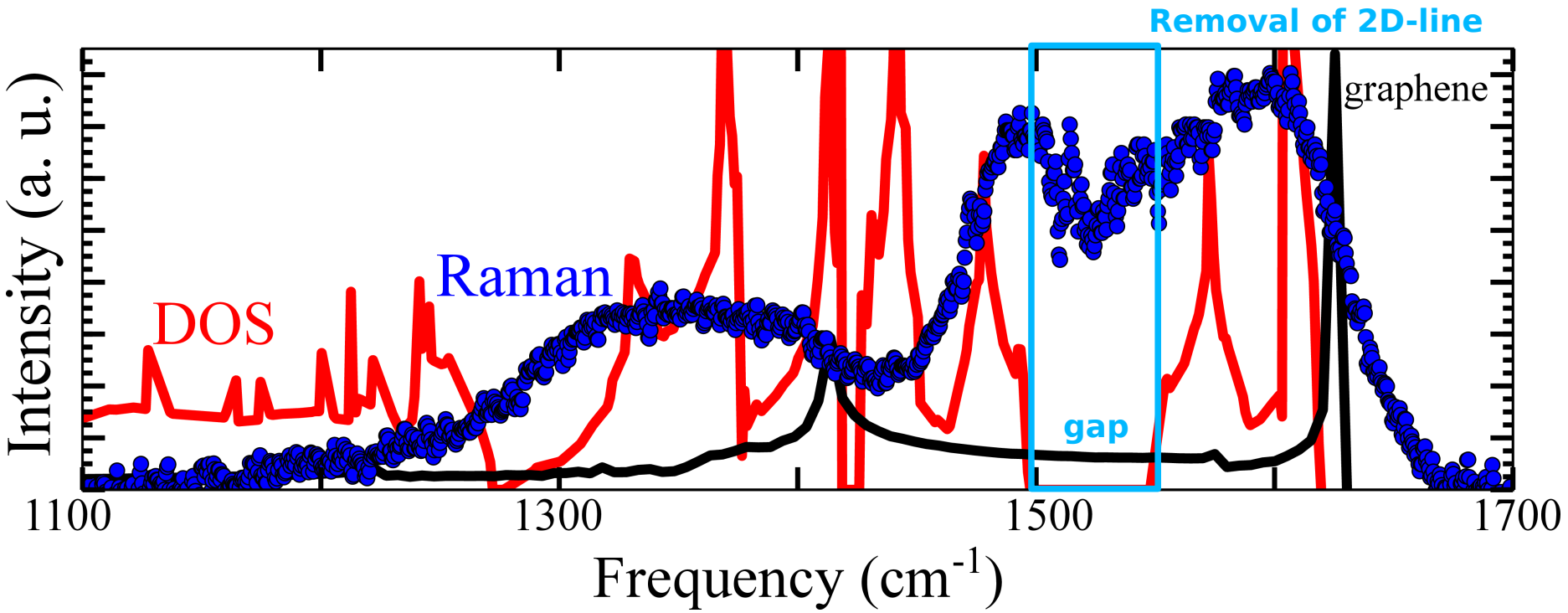
Graphene@SiC. Buffer layer



O. Pankratov et. al. Phys. Rev. B82, 121416R (2010)



Large supercell allows to compare Raman with the density of states

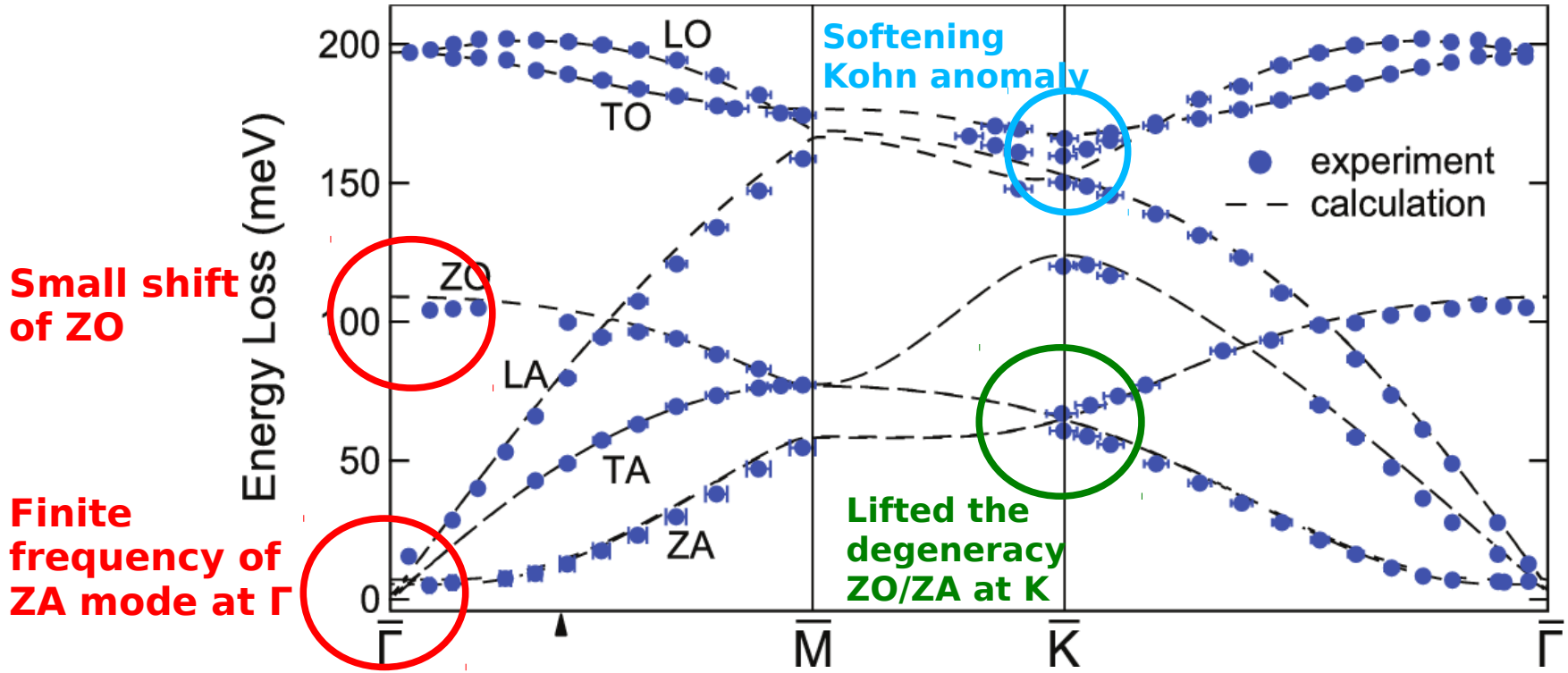


F Fromm, MH Oliveira Jr, AMS et. al., New Journal of Physics, 15 043031 (2013)

Graphene@Iridium(111)

Diffraction spots: long-range Moiré pattern

- Graphene is very detached (d=3.5 nm)
- Lattice parameters are not commensurate.
  Ir(111) = 5.131Bohr, Graphene = 4.630 Bohr
- Formation of Moiré patterns
- EELS experiments: Endlich and Kröger. TU Ilmenau.

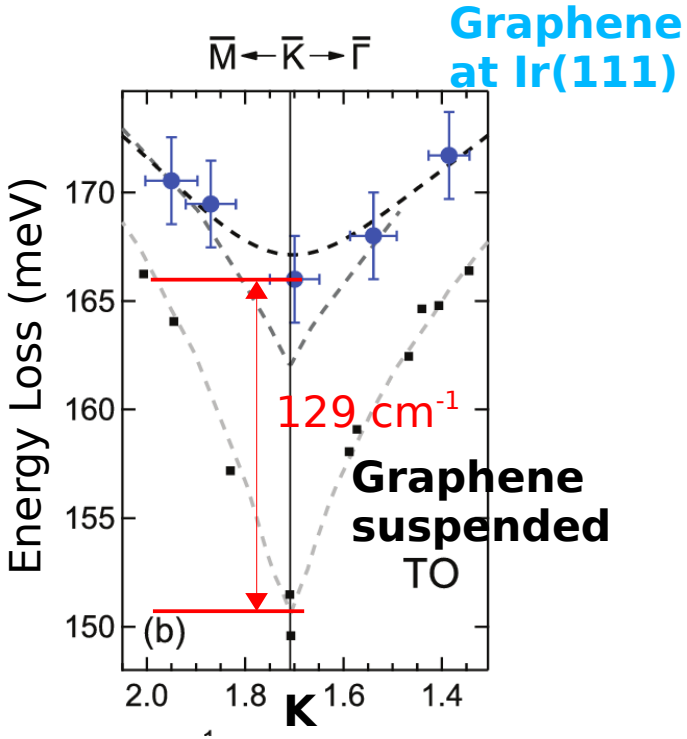


M. Endlich, AMS, L. Wirtz, J. Kröger. Phys. Rev. B 88, 205403 (2013)

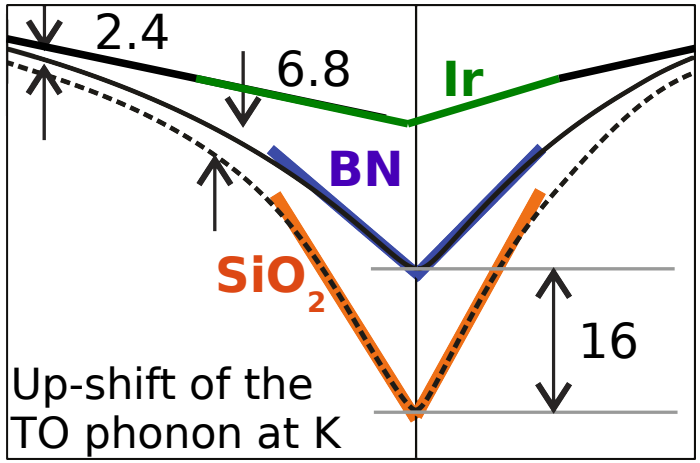
Graphene@Iridium(111)

LDA usually fails to describe TO phonon at K (Kohn anomaly)

Nice agreement with experimental data

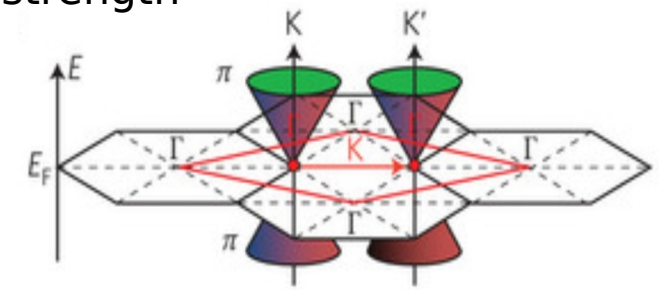


M. Lazzeri et. al., Phys. Rev. B **78**, 081406 (2008)
S. Piscanec et. al., Phys. Rev. Lett. **93**, 185503 (2004)



Comparison with BN up-shift is **129** cm^{-1}!!

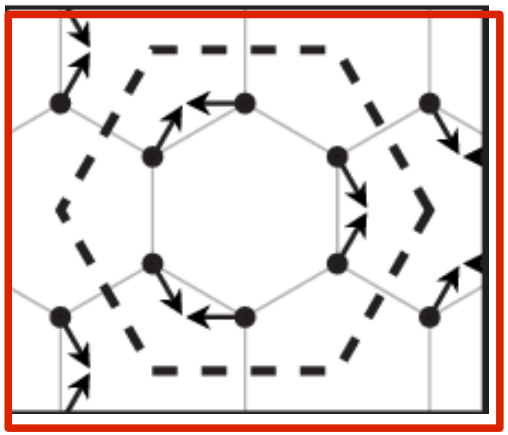
Slope TO branch proportional to electron-phonon coupling strength



F Forster, AMS et. al. Phys. Rev. B 88, 085419 (2013)

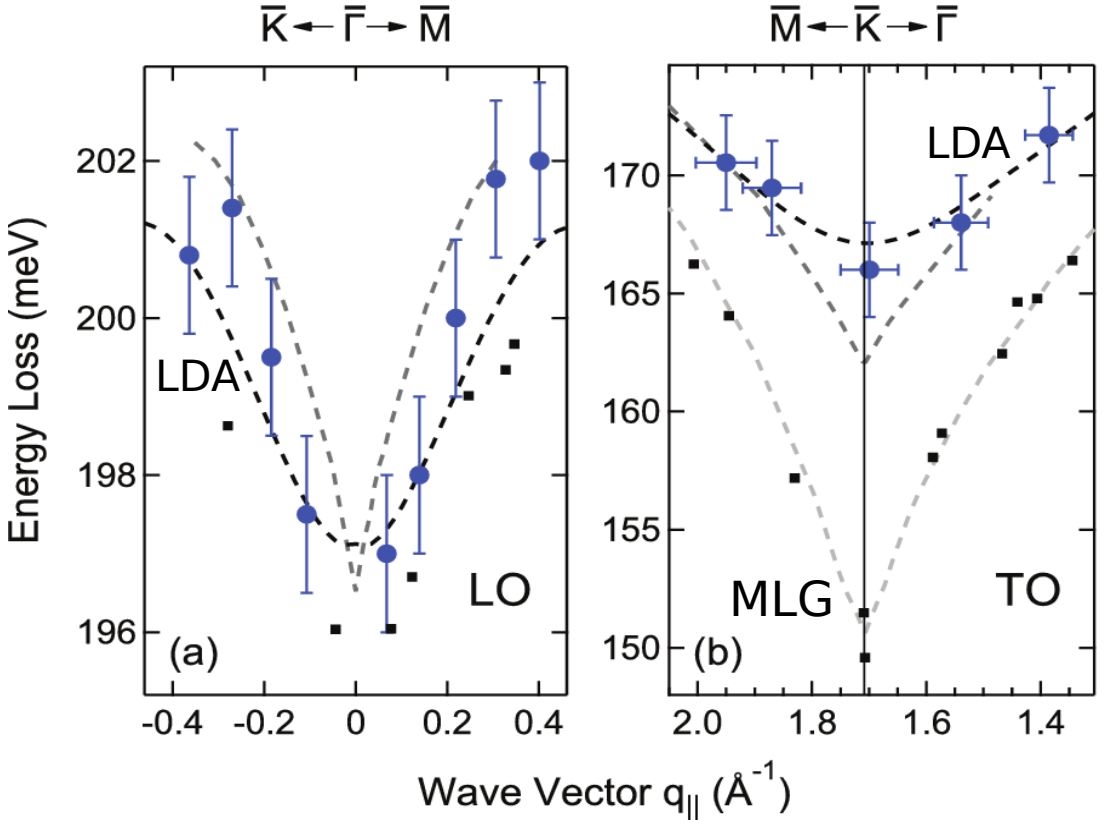
We can calculate el-ph coupling the level of the GW approx.

$$\langle D^2_{\mathbf{K}} \rangle_F = \lim_{d \to 0} \frac{1}{8} \left(\frac{\Delta E_{\mathbf{K}}}{d} \right)^2$$



M. Endlich, AMS, L. Wirtz, J. Kröger. Phys. Rev. B 88, 205403 (2013)

Graphene@Iridium(111)



	graphene	Ir	BN
D_K(LDA)	89.25	89.25	86.00
D_K(GW)	**207.88**	**131.75**	**191.27**

- The metallic screening cancels almost entirely the GW correction.
- This explains the agreement of LDA.
- ZO/ZA at K. Modelling of the corrugation...

M. Endlich, AMS, L. Wirtz, J. Kröger. Phys. Rev. B 88, 205403 (2013)

Summary

	Dirac cone	Screening (main role)	Bonding (main role)
Silicon carbide (buffer layer)	✗	✗	✓
Iridium	✓	✓	✗
Boron nitride	✓	✓	✗

Acknowledgements

- M. Endlich and J. Kröger (TU Ilmenau, DE).
- F. Fromm and T. Seyller (U. Chemnitz, DE).
- F. Forster and C. Stampfer (U. Aachen, DE).

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Summary

Dirac cone **Sc**

Silicon carbide (buffer layer)

Iridium

Boro

Thank you!

ements

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- F. eyller (U. Chemnitz, DE).
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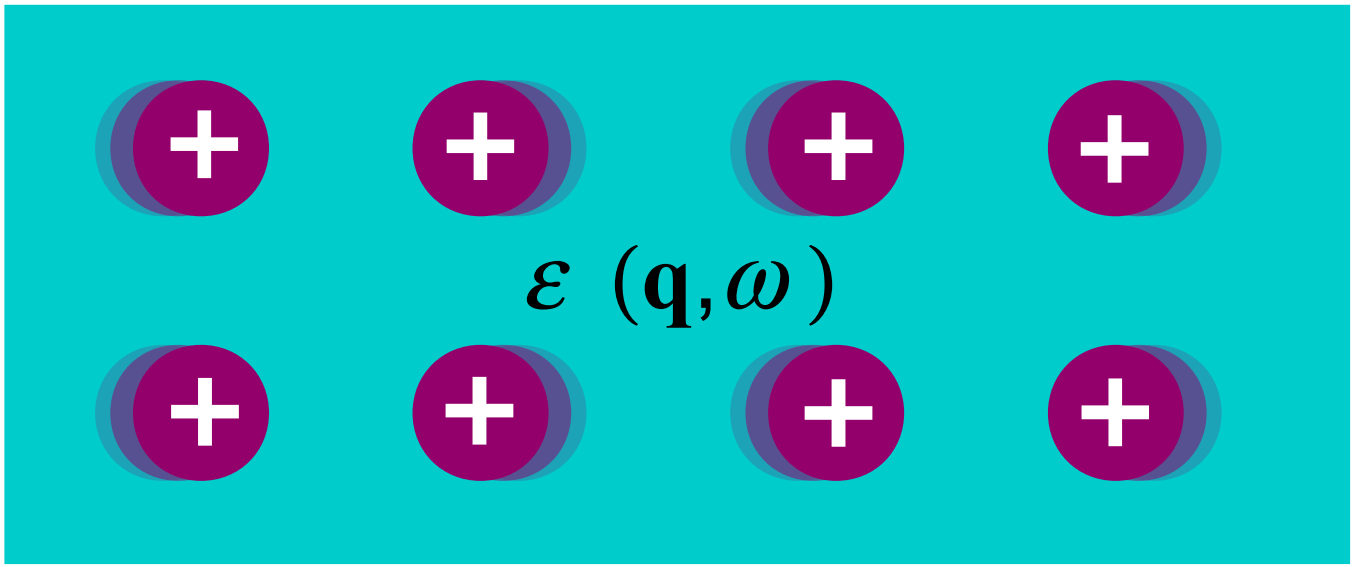
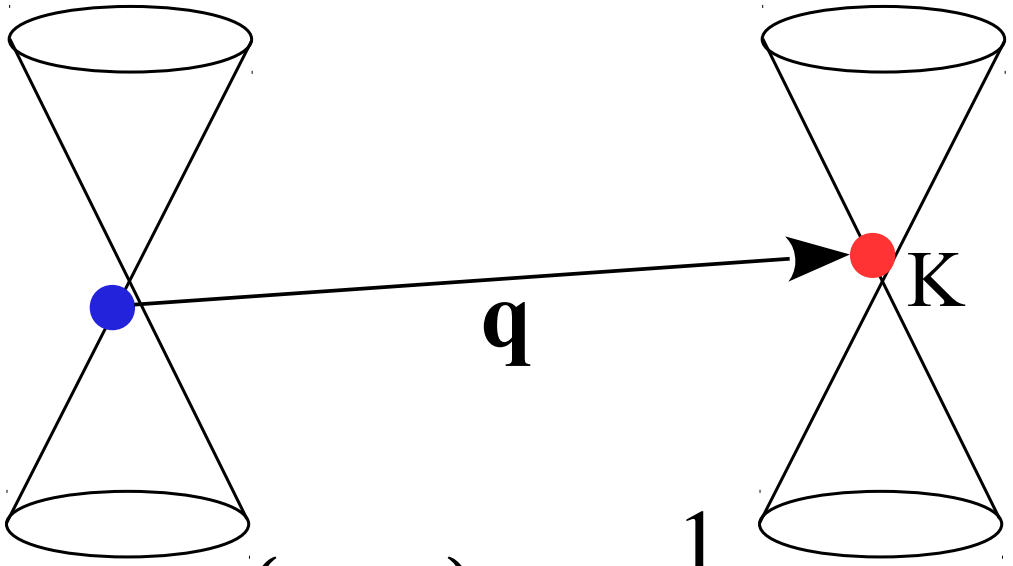
Kohn anomaly





$$\varepsilon(\mathbf{q},\omega) \sim \frac{1}{\varepsilon_c - \varepsilon_v}$$