Interaction of graphene with metallic and semiconductor surfaces. Ab initio approach to the lattice dynamics

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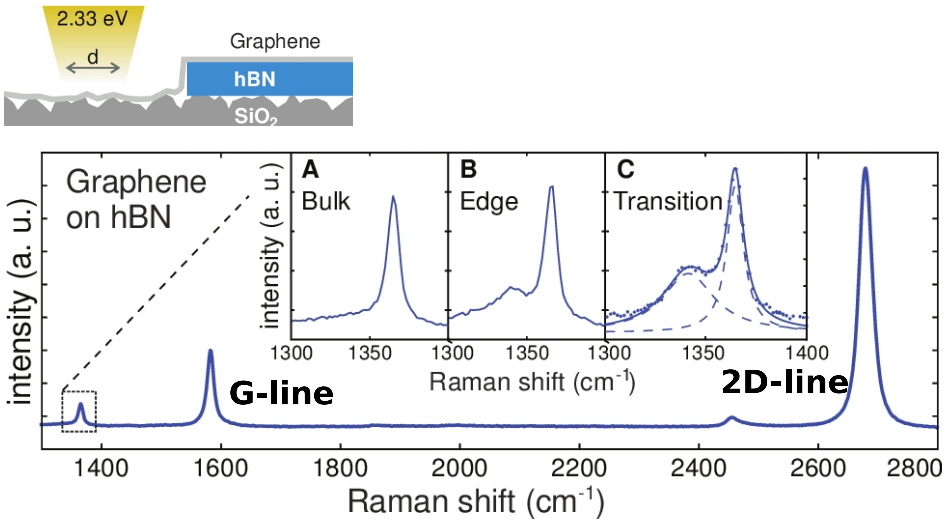
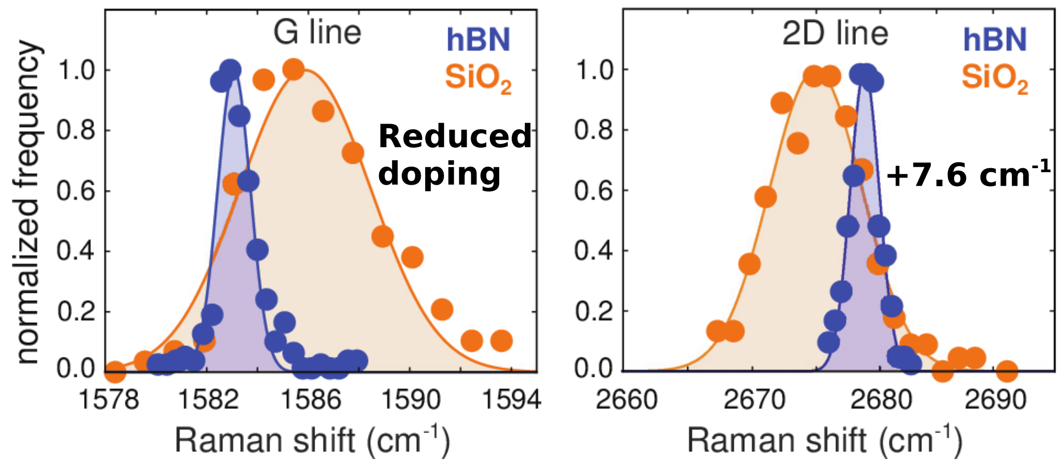
Interaction graphene/substrate

- Graphene has interesting properties
  - Test bench for fundamental physics.
- Response of graphene to the substrate interaction
  - Boron nitride, silicon carbide, iridium.
  - Raman and electron energy loss spectroscopy.
- Lattice dynamics. Density functional theory and GW
  - Attachment graphene/surface.
  - Influence of dielectric screening.
  - Persistence (or not) of some graphene fingerprints (Kohn anomaly, Dirac cone, etc).

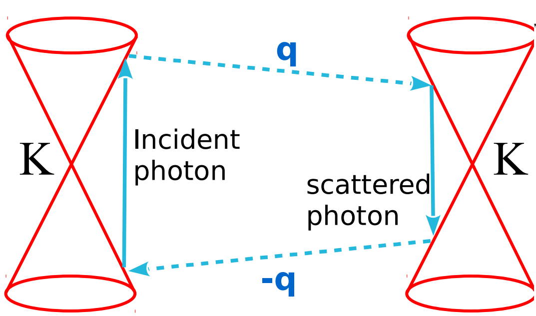
Graphene@BN

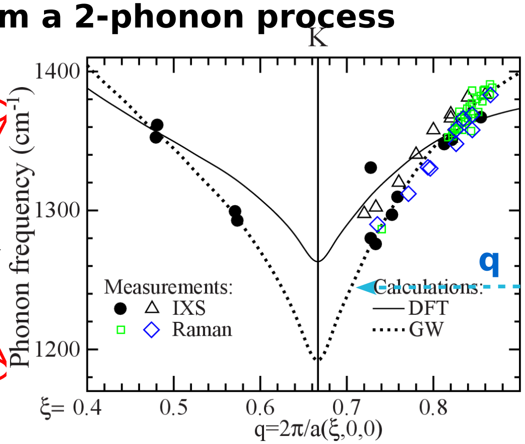
Boron nitride is one of the suitable substrates to keep intrinsic graphene

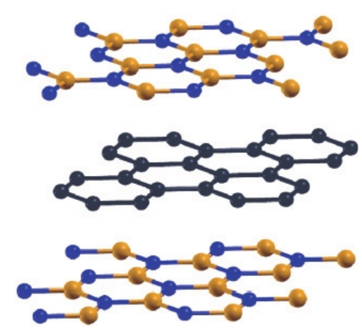




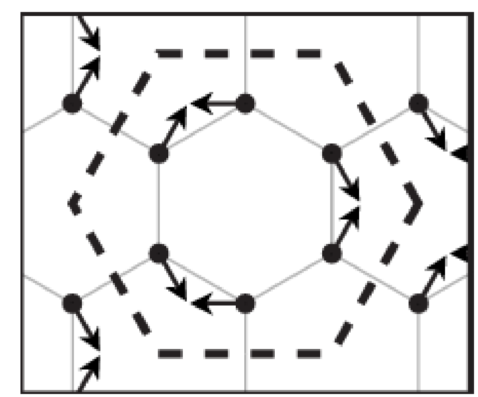
2D-line comes from a 2-phonon process







Calculation in “sandwich” graphene (conserving symmetry)



Slope of the TO phonon at K is proportional to the electron-phonon coupling.
GW approximation must be used.

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

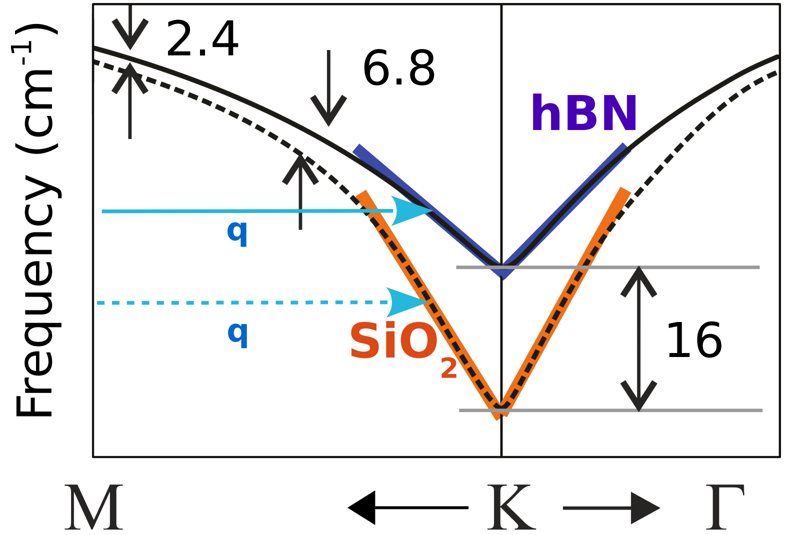
Lazzeri et. al. Phys. Rev. B 78, 081406 (2008)
S. Berciaud et. al., Nano Lett. 10, 4074 (2010)

Phys. Rev. B 88, 085419 (2013)

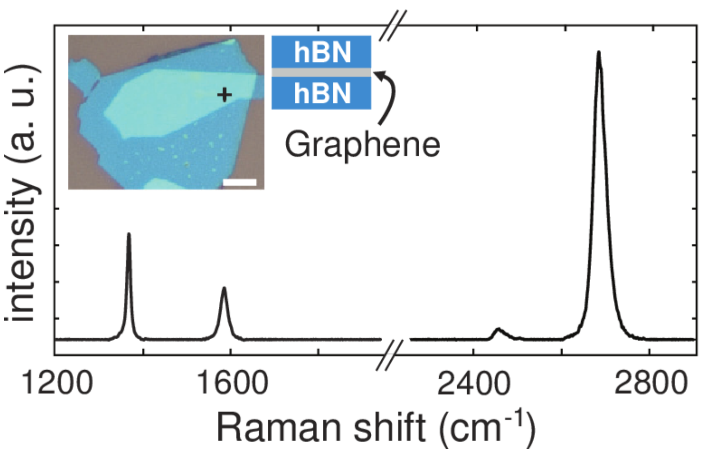
Graphene@BN

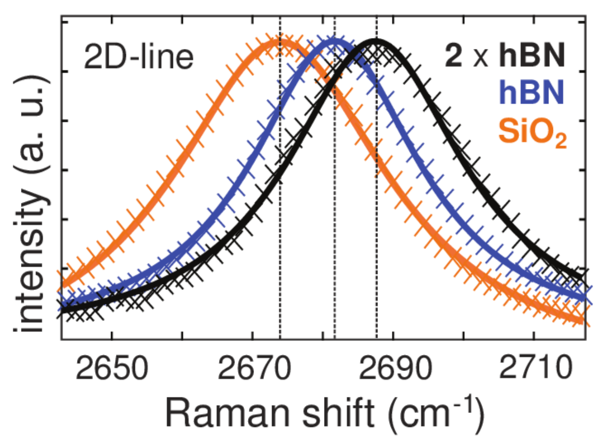
	graphene	on BN
D_{κ}(LDA)	89.25	86.00
D_{κ}(GW)	207.88	191.27

Dielectric screening reduces the bandgap and the strength of the electron-phonon coupling.



- The slope of the optical phonon branch decreases.
- This also explains the down-shift in suspended graphene.
  Nano Lett. 1, 346 (2009).





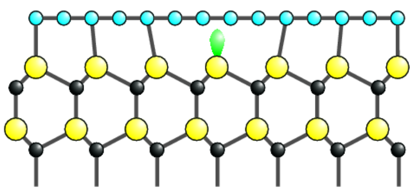
- Our approach can be tested by making a BN-graphene-BN sandwich.
- We observe double up-shift for the 2D-line.

Dielectric screening is the responsible of the up-shift.

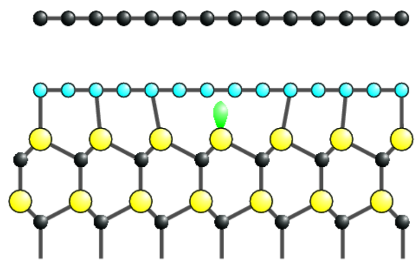
Graphene@SiC. Buffer layer

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

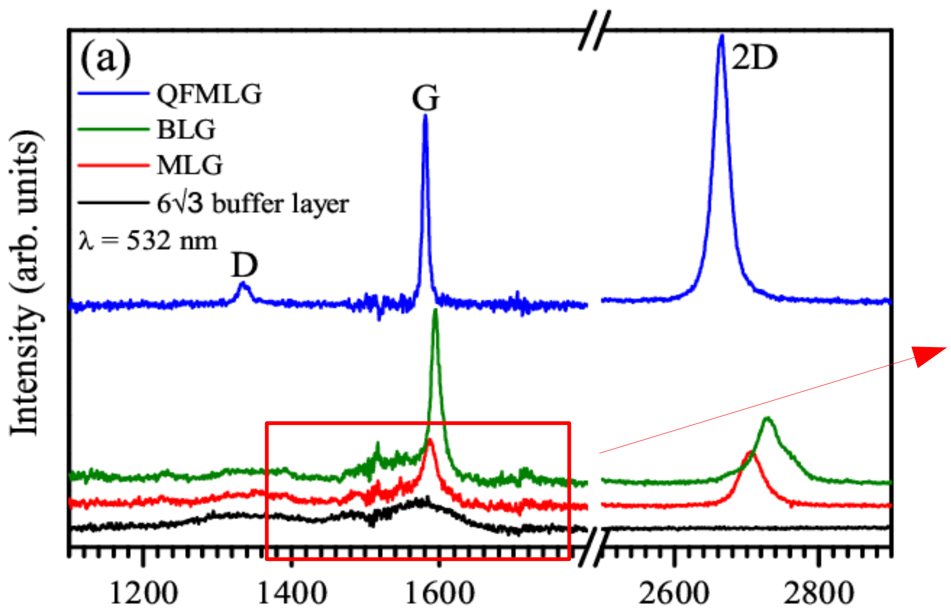
Buffer layer



Epitaxial graphene

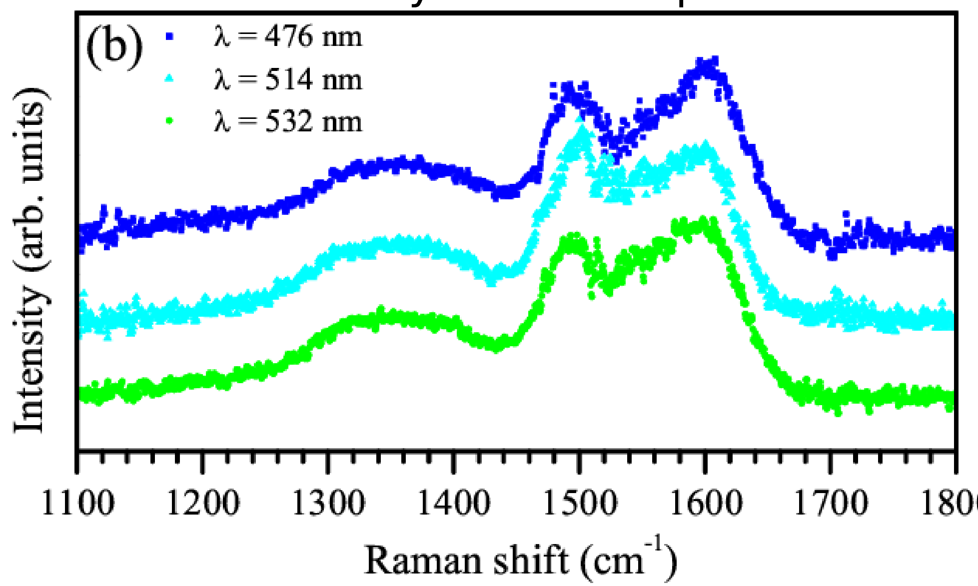


- Hybridization π-states and SiC states.
- Spectra are not compose of discrete peaks.
- Resemble a density of states?



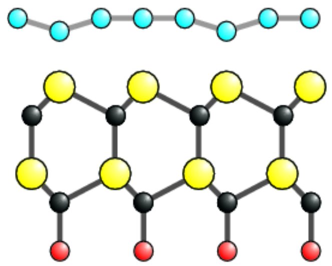
Substraction of SiC spectra

Buffer layer Raman spectra

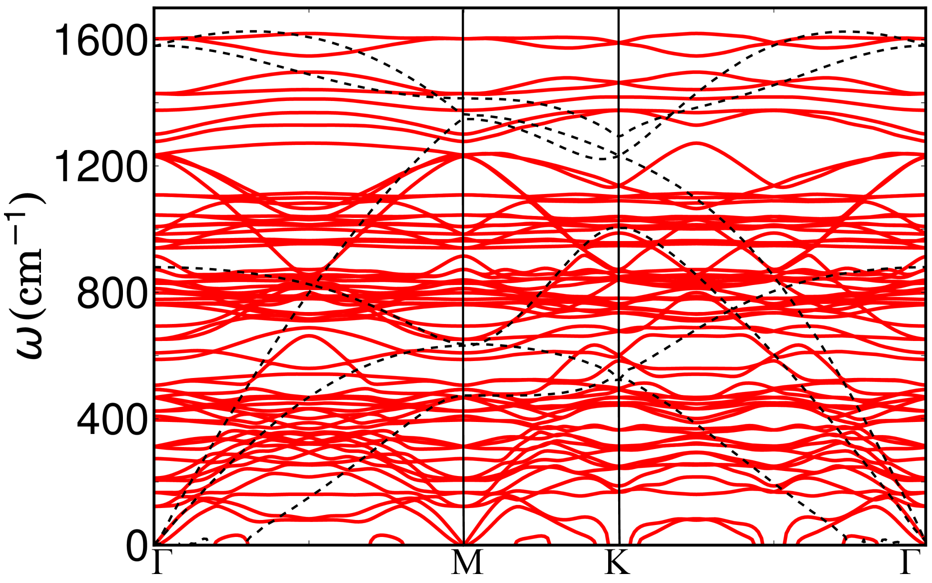


New Journal of Physics, 15 043031 (2013)

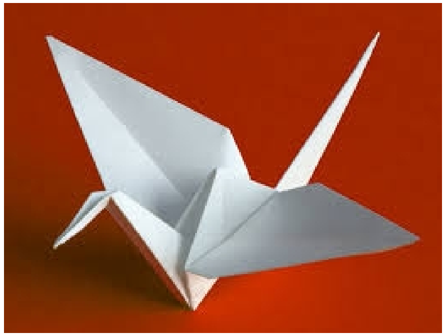
Graphene@SiC. Buffer layer

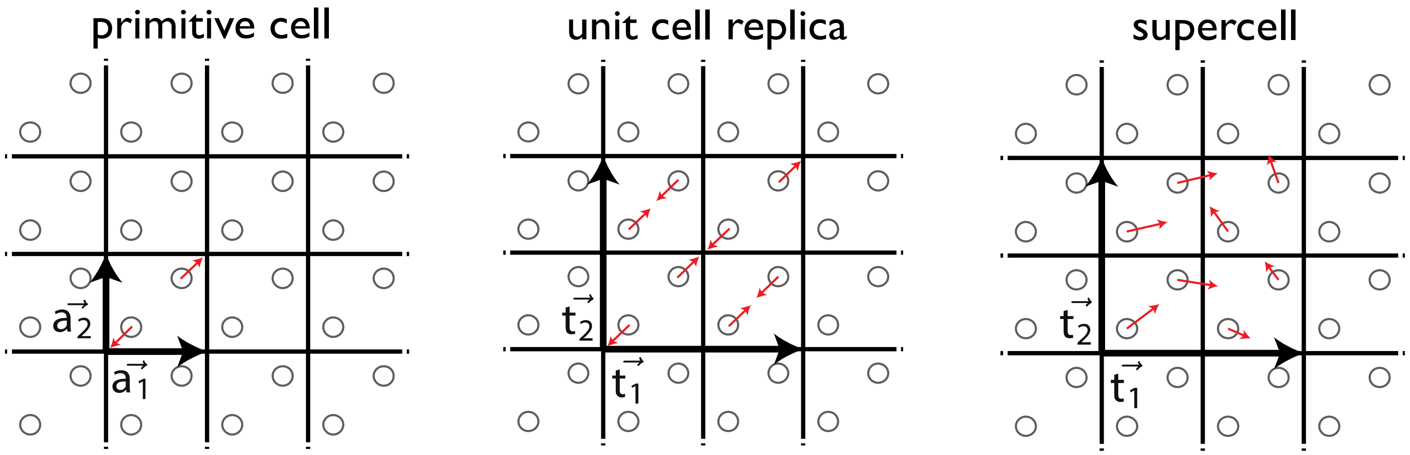


- Strong bonding C-Si: buckling of 0.04 nm
- Large cell to commensurate graphene and SiC

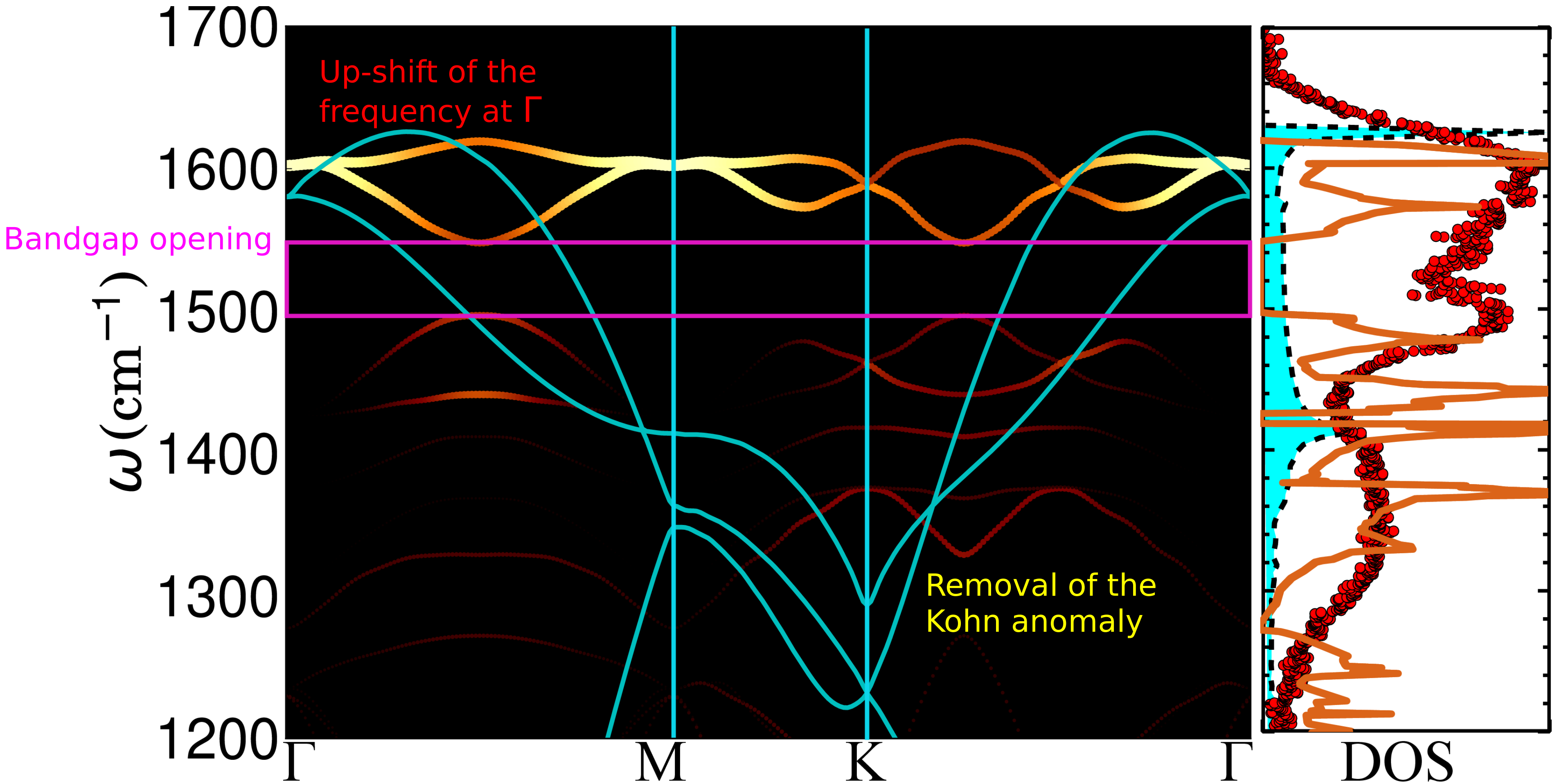


- Performing calculations in large supercells is like an **origami**, we fold the dispersion relation.
- We need to unfold the phonon modes to make easier the interpretation of our results.





Graphene@SiC. Buffer layer

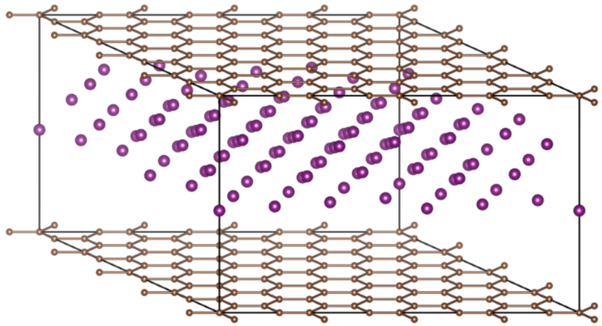


DOS can be compared with Raman spectra

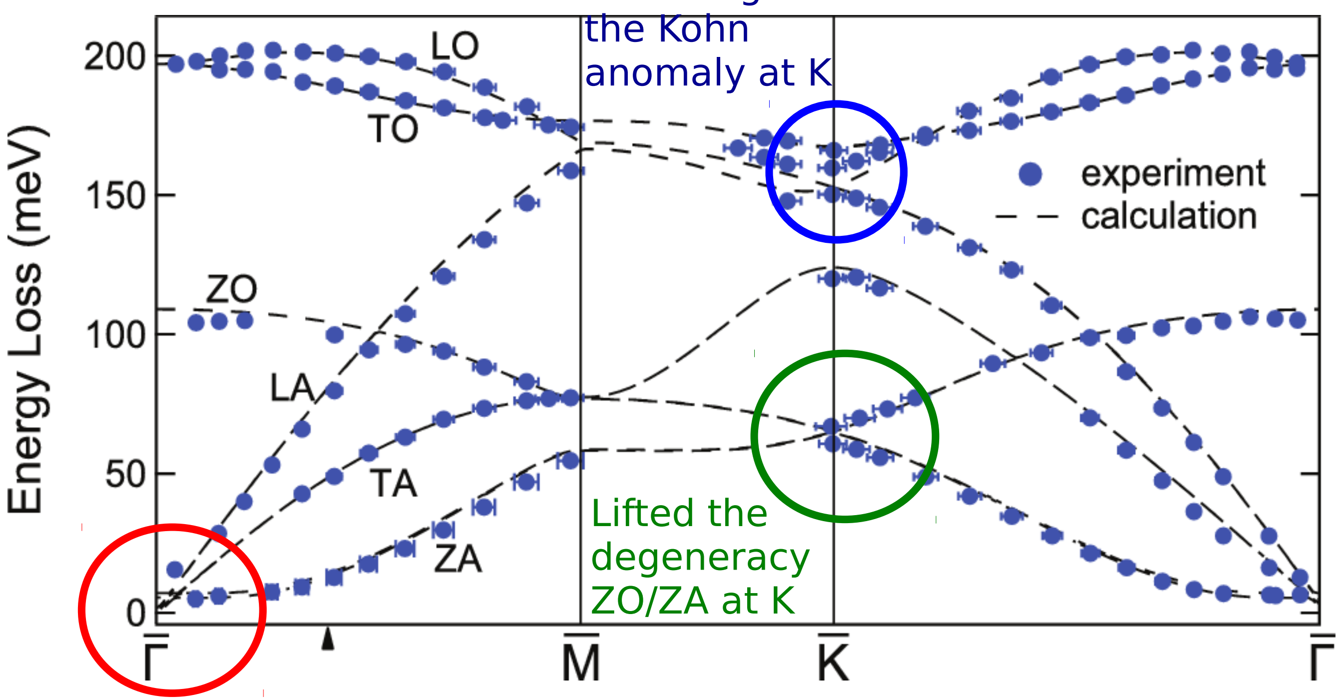
Different with respect to hBN

New Journal of Physics, 15 043031 (2013)

Graphene@Iridium(111)



- 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
- Calculations in large supercells



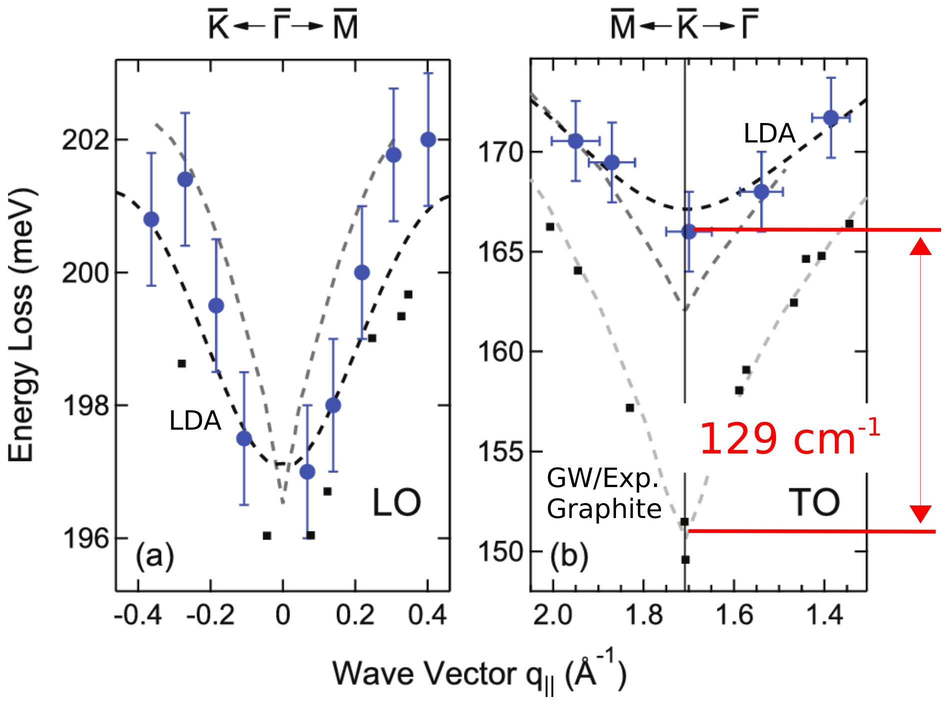
Diffraction spots: long-range Moiré pattern

Calculations performing with LDA.

Graphene unit cell, compressing iridium.

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

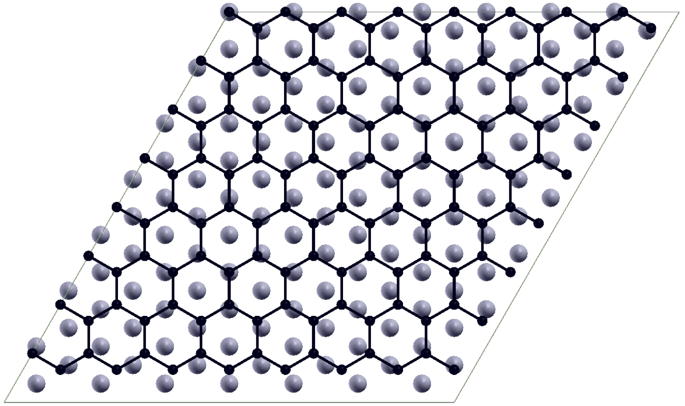
Graphene@Iridium(111)



- LDA calculations in graphene unit cell.
- The metallic screening cancels almost entirely the GW correction.

	graphene	on Ir	on BN
D_κ(LDA)	89.25	89.25	86.00
D_κ(GW)	207.88	131.75	191.27

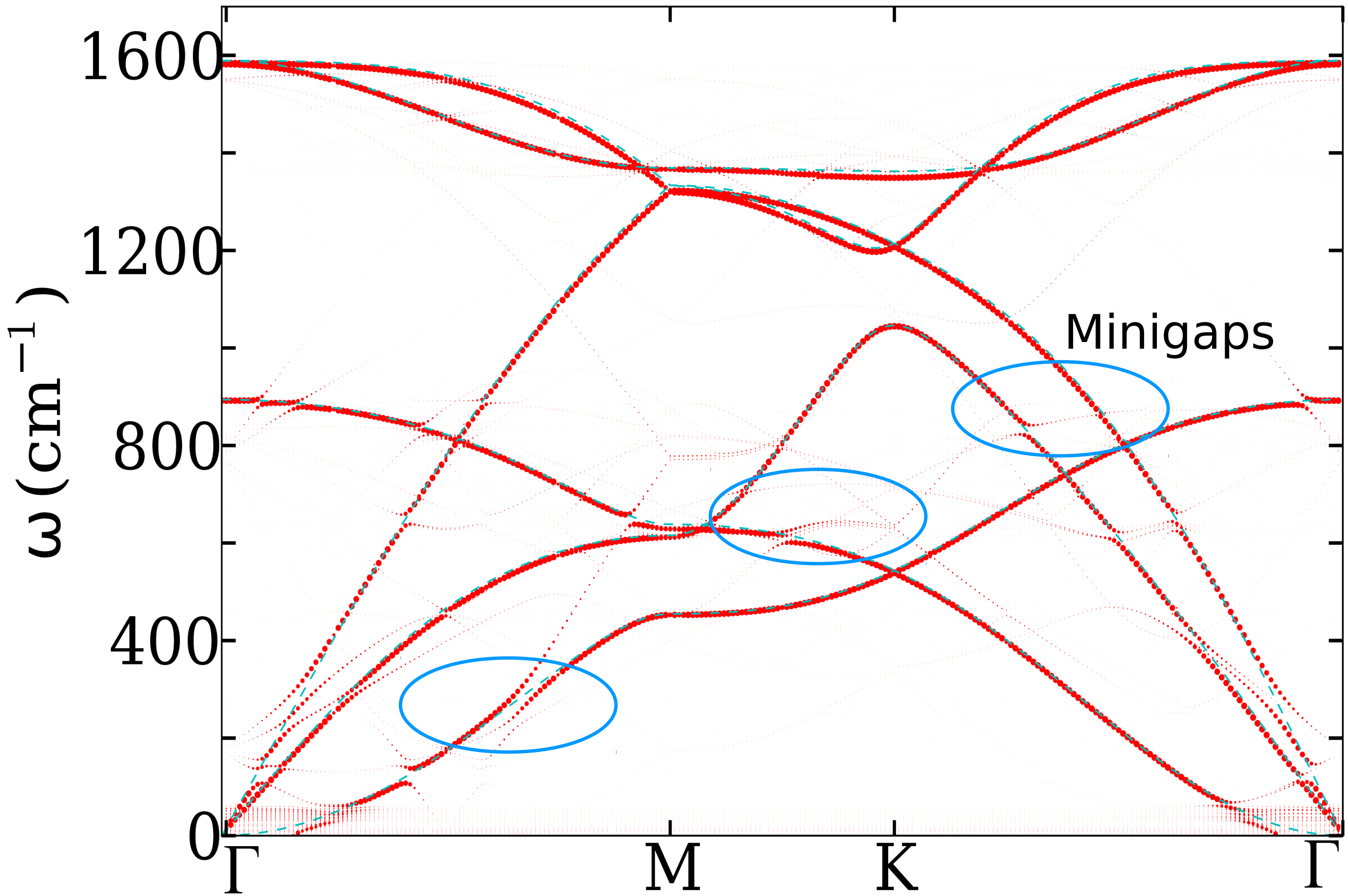
- Variation of the local environment produces a corrugation in graphene.
- Number of atoms in unit cell exceeds the limit of application of ab-initio methods.
- Empirical methods. Force constant model.



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

Graphene@Iridium(111)

Preliminar results for a 8x8-graphene unit cell (177 atoms)



Corrugation is still missing in the modeling

Graphene phonon bands are almost unchanged

Conclusions and future work

- Lattice dynamics gives valuable information about attachment of graphene, screening, and conservation of intrinsic properties.

Acknowledgements

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Conclusions and futur

Thank you!

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- ...pfer (U. Aachen, DE).
- M. ... u J. Kröger (TU Ilmenau, DE).

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