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

Alejandro Molina-Sánchez, Henrique Miranda and Ludger Wirtz
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).
Boron nitride is one of the suitable substrates to keep intrinsic graphene.

Graphene@BN

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

S. Berciaud et. al., Nano Lett. 10, 4074 (2010)
Graphene@BN

| graphene on BN |  
|----------------|----------------|
| $D_K$(LDA)     | 89.25          |
| $D_K$(GW)      | 207.88         |

**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).

**Dielectric screening is the responsible of the up-shift.**

![Graphene spectrum and optical phonon branch](image)
Graphene@SiC. Buffer layer

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

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

Buffer layer Raman spectra

Subtractions of SiC 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

Bandgap opening

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.
  \( \text{Ir}(111) = 5.131\text{Bohr}, \text{Graphene} = 4.630\text{ Bohr} \)
- Formation of Moiré patterns
- Calculations in large supercells

---

Finite frequency of ZA mode at  \( \Gamma \)

Diffraction spots: long-range Moiré pattern

Calculations performing with LDA.

Graphene unit cell, compressing iridium.

Graphene@Iridium(111)

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

<table>
<thead>
<tr>
<th></th>
<th>graphene on Ir</th>
<th>on BN</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_K$(LDA)</td>
<td>89.25</td>
<td>89.25</td>
</tr>
<tr>
<td>$D_K$(GW)</td>
<td>207.88</td>
<td>131.75</td>
</tr>
</tbody>
</table>

- 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.

Graphene@Iridium(111)

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

Minigaps

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

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

Acknowledgements

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

Thank you!