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

Alejandro Molina-Sánchez,
Henrique Miranda and Ludger Wirtz

Physics and Materials Science Research Unit
University of Luxembourg
Interaction graphene/substrate

The physical properties of graphene depend critically on the environment.

Change in phonon modes allows to characterize graphene/substrate interaction.

Ab-initio calculations of the lattice dynamics

silicon carbide


iridium


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.

Graphene@SiC. Buffer layer

Buffer layer Raman spectra

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

Spectra are not composed of discrete peaks.

Resemble a density of states?

Experimental data from F Fromm & T. Seyller

Graphene@SiC. Buffer layer

Calculations in a 2x2 graphene unit cell.

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

Graphene@SiC. un-folding
Graphene@SiC. Buffer layer

Graphene@SiC. Buffer layer

Large supercell allows to compare Raman with the density of states

Removal of 2D-line


Graphene@Iridium(111)

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

Diffraction spots: long-range Moiré pattern

Small shift of ZO

Finite frequency of ZA mode at $\Gamma$

Graphene@Iridium(111)

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

Nice agreement with experimental data

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

\[
\langle D_K^2 \rangle_F = \lim_{d \to 0} 8 \left( \frac{\Delta E_K}{d} \right)^2
\]

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

Slope TO branch proportional to electron-phonon coupling strength


The metallic screening cancels almost entirely the GW correction.

This explains the agreement of LDA.

ZO/ZA at K. Modelling of the corrugation...

---

<table>
<thead>
<tr>
<th></th>
<th>graphene</th>
<th>Ir</th>
<th>BN</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_K$(LDA)</td>
<td>89.25</td>
<td>89.25</td>
<td>86.00</td>
</tr>
<tr>
<td>$D_K$(GW)</td>
<td><strong>207.88</strong></td>
<td><strong>131.75</strong></td>
<td><strong>191.27</strong></td>
</tr>
</tbody>
</table>
Summary

<table>
<thead>
<tr>
<th></th>
<th>Dirac cone</th>
<th>Screening (main role)</th>
<th>Bonding (main role)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Silicon carbide</td>
<td>✗</td>
<td>✗</td>
<td>✓</td>
</tr>
<tr>
<td>(buffer layer)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Iridium</td>
<td>✓</td>
<td>✓</td>
<td>✗</td>
</tr>
<tr>
<td>Boron nitride</td>
<td>✓</td>
<td>✓</td>
<td>✗</td>
</tr>
</tbody>
</table>

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).
Summary

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

Acknowledgements

Dirac cone (main role)
Screening
Bonding (main role)
Silicon carbide (buffer layer)
Iridium

Thank you!
Kohn anomaly

\[ \varepsilon(q, \omega) \sim \frac{1}{\varepsilon_c - \varepsilon_v} \]