Infrared spectroscopy of vertical heterostructures of graphene and hexagonal boron nitride

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March 15th, 2016
1.8% lattice mismatch
Possible angular misalignment
Moiré pattern forms

Properties of \textit{vertical heterostructures} depend entirely on the nature of inter-layer interactions
These are difficult to predict in theory

\begin{align*}
u_0 &= -0.15, \ u_1 = 0, \ u_3 = 0 \\
u_0 &= 0, \ u_1 = 0.075, \ u_3 = 0.075
\end{align*}

Optical spectroscopy can reveal details about inter-layer interactions

- 1.8% lattice mismatch
- Possible angular misalignment
- Moiré pattern forms

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Interpretation of the interaction

\[
V = (u_0^+ f_+ + u_0^- f_-) + \tau_z \sigma_z (u_3^+ f_- + u_3^- f_+) \\
+ \tau_z \sigma \cdot [l_z \times \nabla (u_1^+ f_- + u_1^- f_+)] + \Delta \tau_z \sigma_z.
\]

\[
f_+ = \sum_n e^{i b_n \cdot r}, \quad f_- = i \sum_n (-1)^n e^{i b_n \cdot r}
\]

<table>
<thead>
<tr>
<th>Physical interpretation</th>
<th>Inversion symmetric</th>
<th>Inversion antisymmetric</th>
</tr>
</thead>
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<tr>
<td>Potential modulation</td>
<td>$u_0^+$</td>
<td>$u_0^-$</td>
</tr>
<tr>
<td>Modulation of hopping</td>
<td>$u_1^+$</td>
<td>$u_1^-$</td>
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<td>Local sublattice asymmetry</td>
<td>$u_3^+$</td>
<td>$u_3^-$</td>
</tr>
<tr>
<td>Global sublattice asymmetry</td>
<td>$\Delta$</td>
<td></td>
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</table>

Predictions exist in the literature
Effect of individual terms

- For strong $u_0$, double peak structure from mBZ edge reconstruction.
- For strong $u_1$, dip–peak–peak.
- For strong $u_3$, peak–dip–peak.

Comparison to existing theory

Model 1 | Point charge lattice | [1]
Model 4 | DFT + elastic theory | [2]


Summary

- **Infra-red spectroscopy** a key tool for understanding van der Waals interactions in 2D heterostructures.

- Clearest diagnostics found by **sweeping density** through first miniband


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