### Introduction

Graphene has some interesting properties:
- high charge-carrier mobility
- the ballistic electron transport at room temperature
- (...)

Practical applications: Interaction with a substrate
- Ir(111) and Pt(111) good candidates, large separation and weak interaction

Aim of the project:
- Create a force-constant model of graphene on Ir(111)
- Implement the model in a code
- Predict the phonon-dispersion
- Explain the characteristics of the phonon dispersion

### Experimental Phonon dispersion of graphene on Ir(111)

Obtained using high resolution electron energy loss spectroscopy (HREELS precision of ±4meV [1])

#### Force constant model

Force constant matrix of the interaction (local coordinates) of two atoms, depends on:
- Types of atoms interacting,
- Distance between them (using cubic splines).

Transform to global coordinates:

\[
C_{ij} = \left[ \begin{array}{c|c} C_{aa} & C_{ab} \\ \hline C_{ba} & C_{bb} \end{array} \right]
\]

Build the dynamical matrix:

\[
D_{ij}(k) = \frac{1}{V} \sum_{r \in \Omega} C_{ijijkl} \exp(ik \cdot r)
\]

Calculate the phonon frequencies:

\[
\det\left[D_{ii}(k) - \omega^2(k)I\right] = 0
\]

### Folding of the phonon dispersion

#### Results

1. Find correspondence between the atoms of the supercell and the unit cell
2. Construct replicas of the unit cell with the size of the supercell
3. Project the phonons of the replica of the primitive cell in the supercell

#### Force constant model

For graphene on Ir(111):

\[
C_{ij} = \left[ \begin{array}{c|c} C_{aa} & C_{ab} \\ \hline C_{ba} & C_{bb} \end{array} \right]
\]

#### References