TECHNISCHE UNIVERSITÄT CHEMNITZ

Structural and electronic investigations of Bismuth multilayers

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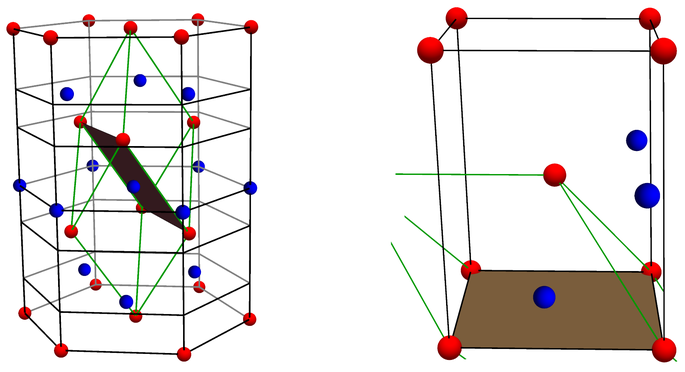
Bulk bismuth structure

- Rhombohedral unit cell with 2-atomic basis (green)
- $\alpha_\rho = 58.7 \rightarrow$ slightly distorted fcc lattice
- Bi (111) unit cell: hexagonal double-layer structure (red/blue spheres)
- Bi (110) unit cell: orthorhombic structure

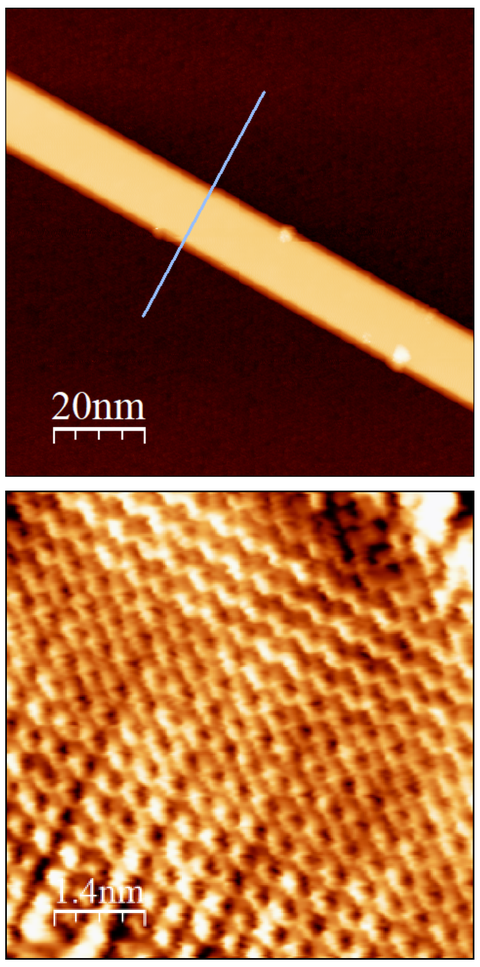


Experiments of Bi (110) on graphene

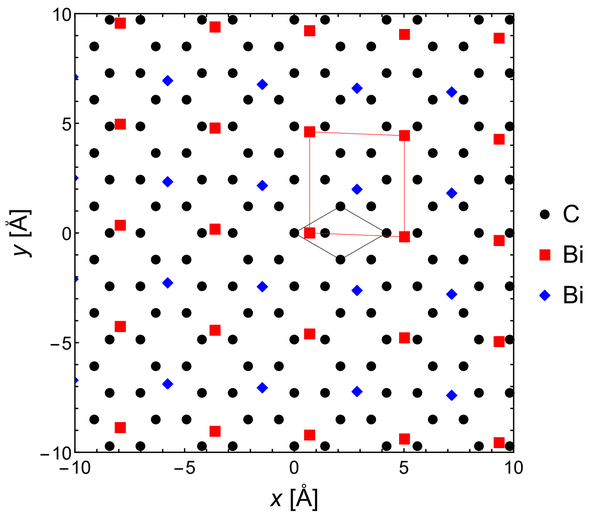
- Bismuth (110) growth on graphene on Si substrate
- Different numbers of multilayers found (> 3)
- Lattice constants from diffraction pattern:

  Graphene: hexagonal
  $a_{Gr} = 2.43$ Å
  Bismuth: monoclinic
  $a_1 = 4.32$ Å , $a_2 = 4.61$ Å , $\alpha = 92.29°$

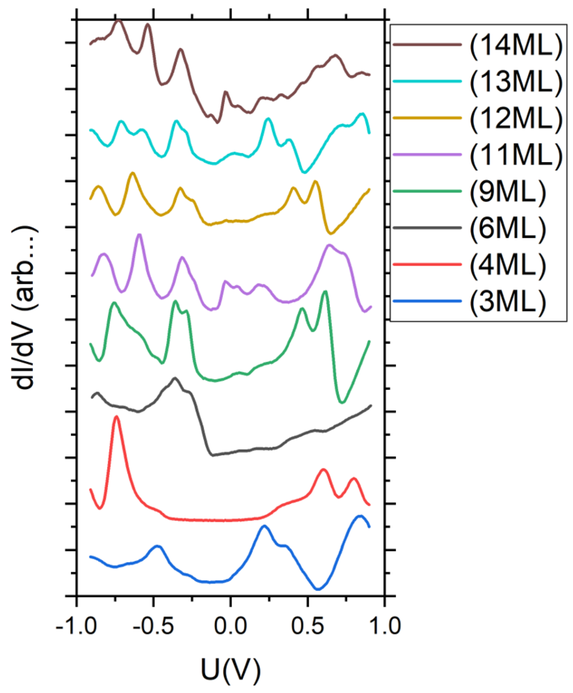
Scanning tunneling microscopy (STM) images:



Structure model:



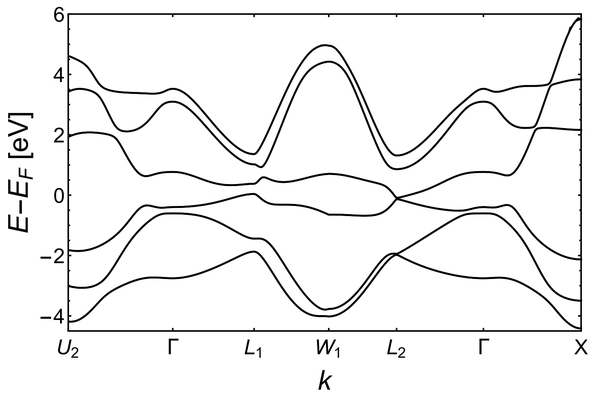
Differential conductance:



Calculational details

- Density functional theory (DFT)
- Software: Abinit
- Plane wave basis
- Exchange-correlation functional: GGA-PBE
- Pseudopotential: Hartwigsen-Goedecker-Hutter (HGH)
- Electron configuration of $_{83}$Bi: [He] $4f^{14}\ 5d^{10}\ 6s^2\ 6p^3$
- 5 valence electrons: $6s^2\ 6p^3$
- Spin + spin-orbit coupling (SOC) included
- Energy cutoff: 20 Ha
- K point grid: $8^d \ldots 16^d$ (d . . . dimension)

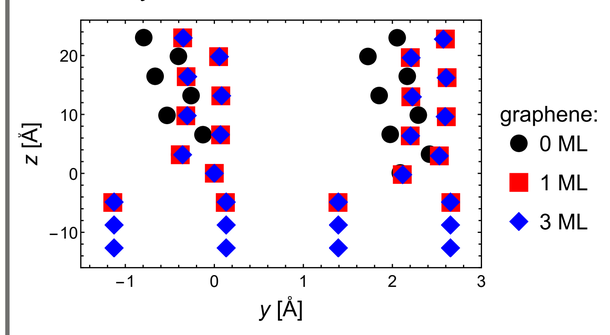
Bulk Bi bandstructure:

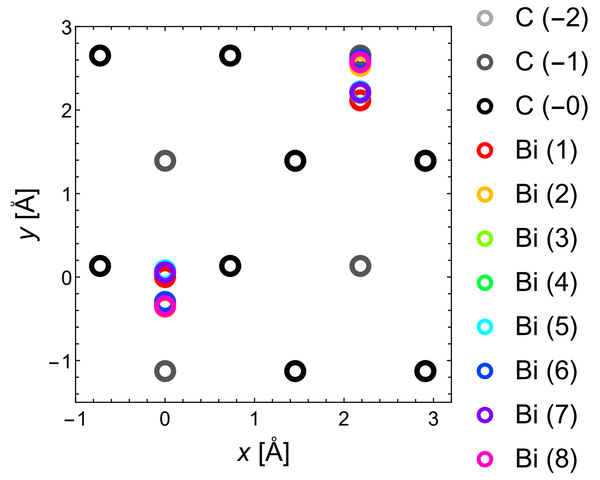


$\rightarrow$ consistent with Phys Rev. B 91 (2015) 125129

Calculations of Bi (110): structural properties

- Orthorhombic structure
- Cell: 2× Bi / 8× C per layer
- 6% tension compared to bulk calculation
- 1 Bi layer unstable



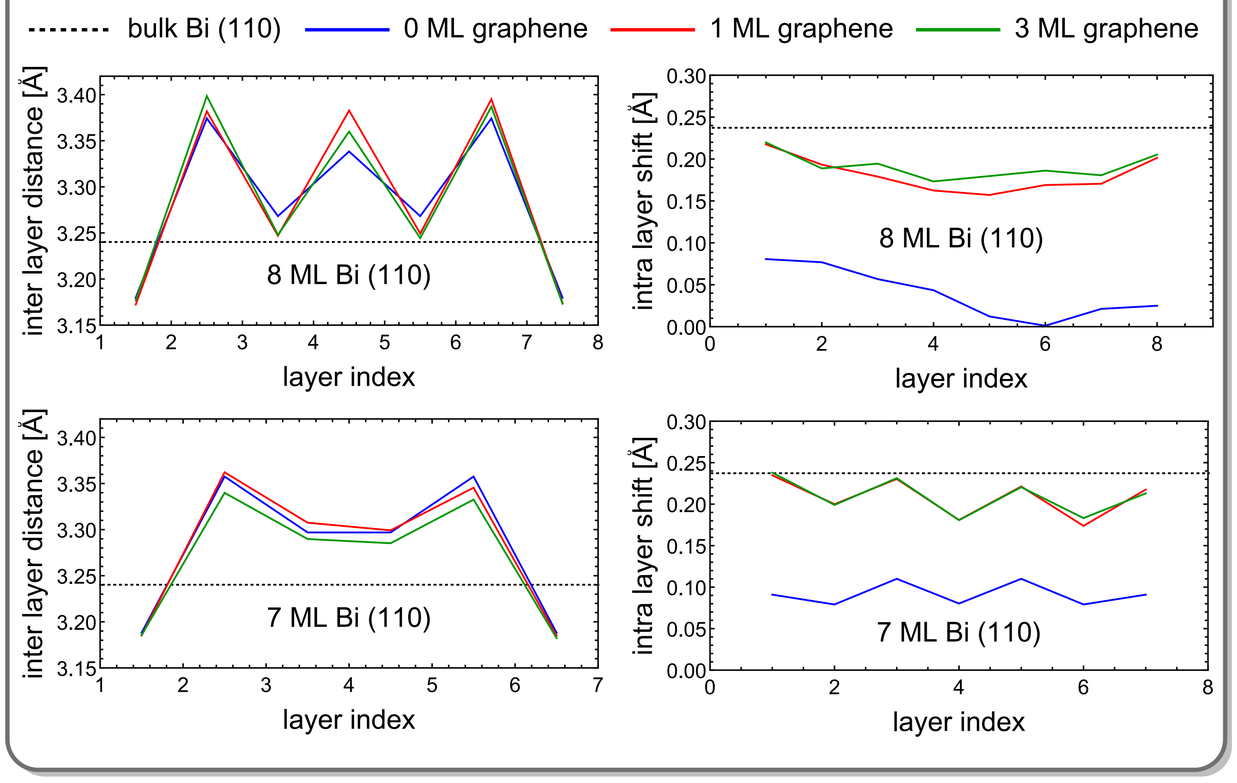


Inter layer distances:

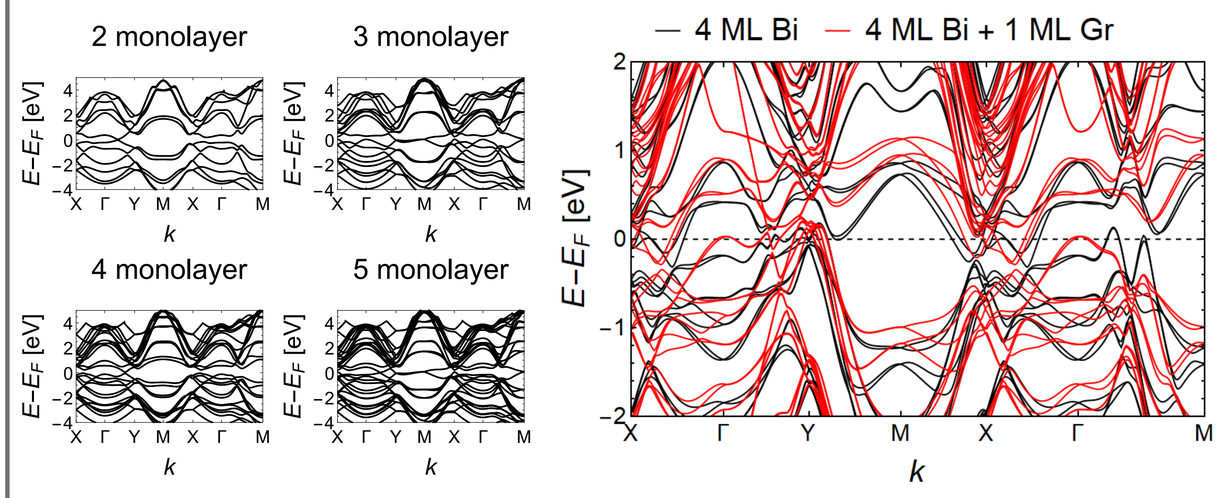
- Enhanced comparing bulk Bi
- Even/odd effect concerning number of layers
- Even/odd effect concerning layer number

Intra layer shifts:

- Strongly reduced for Bi without graphene
- Slightly reduced for Bi on graphene
- Even/odd effect



Calculations of Bi (110): electronic properties

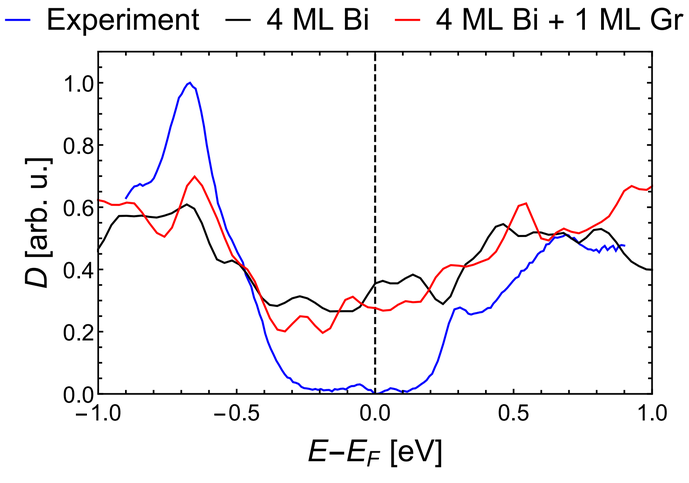


Bandstructure:

- Even/odd effects
- With 1 ML graphene:
  Graphene bands lowered in energy
  Bi states increased in energy
- Charge transferred from Bi to graphene

Density of states:

- HOMO peaks fit experiment
- LUMO peak fit better for 1 ML graphene
- Bandgap missing



Conclusion

- Structure calculations: even/odd effects, but no black phosphorus lattice
- Bandstructure: charge transferred from Bi to graphene
- Density of states: HOMO/LUMO peaks fit, bandgap missing