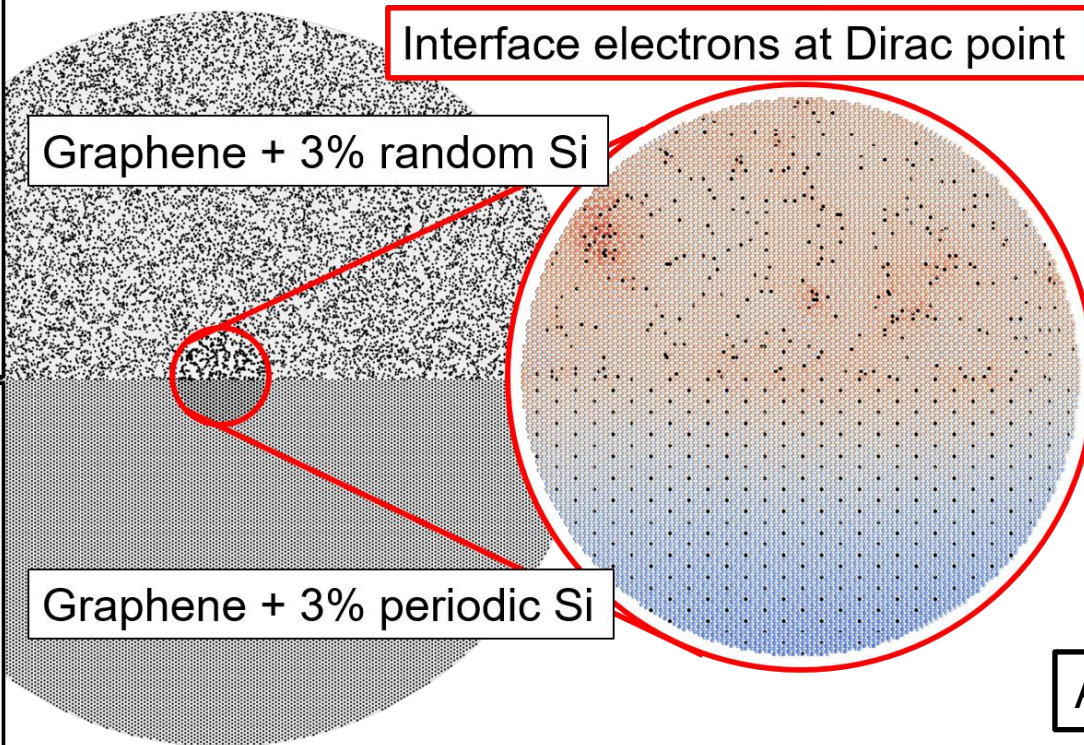
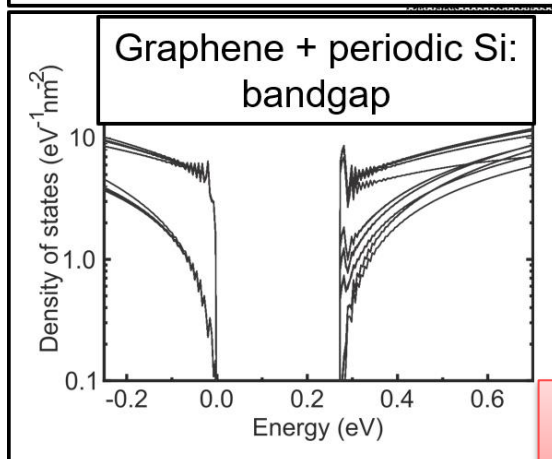
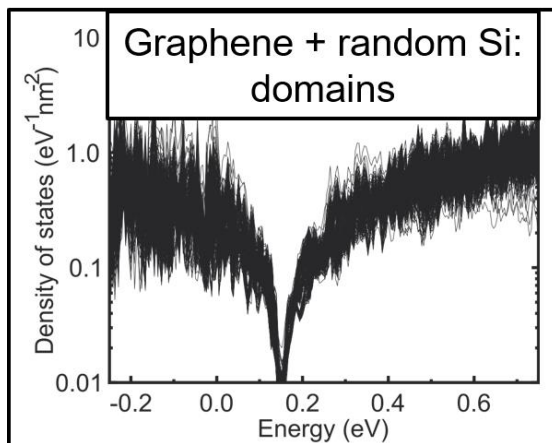


Highlight ROBIN: example of Si doping in graphene

ROBIN – recursive open boundary and interfaces method

General: regular and irregular systems; Fast: handles millions of atoms



Quantitative agreement with experiment:
3% Si in graphene shifts work function by 147 meV

“All around contact”
Door opener to explicit interface modeling

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Periodicity vs. irregularity gives systematic material change
ROBIN is first the first method to model irregular atom distributions