APS March Meeting

Ab Initio Theory of Gate Induced Gaps in Graphene Bilayers

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Outline

We study the gate voltage induced gap in graphene bilayers using *ab initio* density functional theory. Our calculations confirm the qualitative picture suggested by phenomenological tight-binding models. We discuss screening of the external potential and quantify the role of crystalline inhomogeneity using a tight-binding self-consistent Hartree calculation.

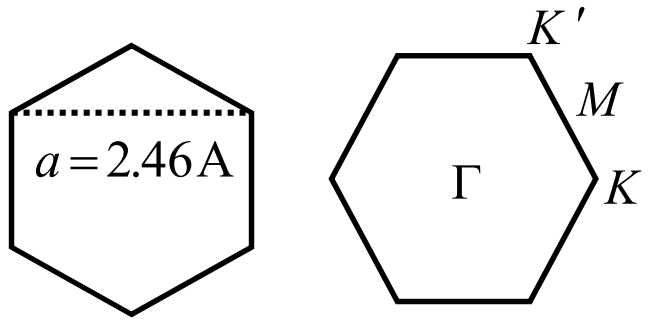
1. Introduction
2. *Ab initio* Calculations
3. Self-consistent Hartree Calculations

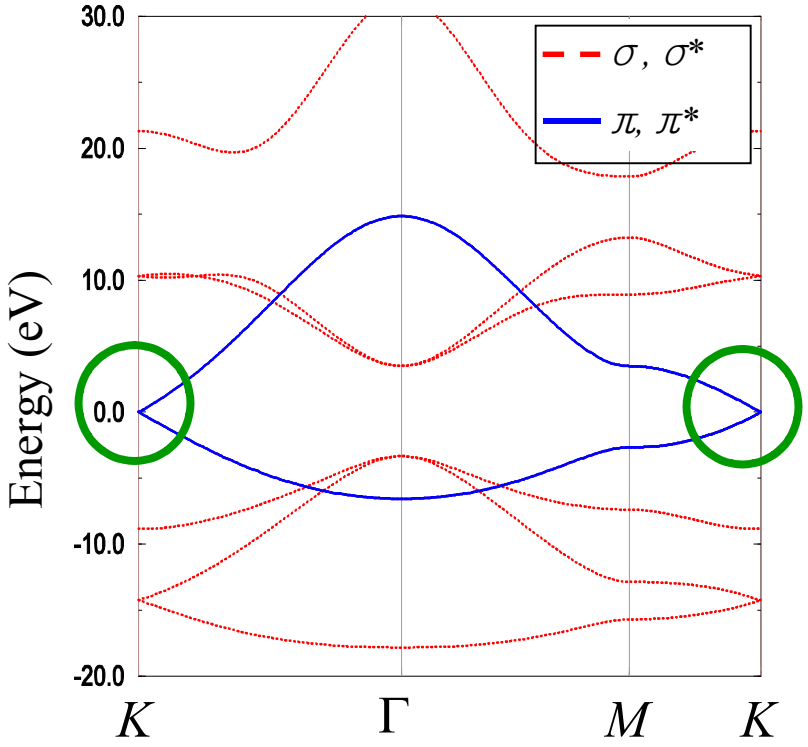
1. Introduction

1) Graphene

- Graphene is a two-dimensional honeycomb lattice of carbon atoms.

- Energy bands at low energies are described by a 2D Dirac-like equation with linear dispersion near K/K'.

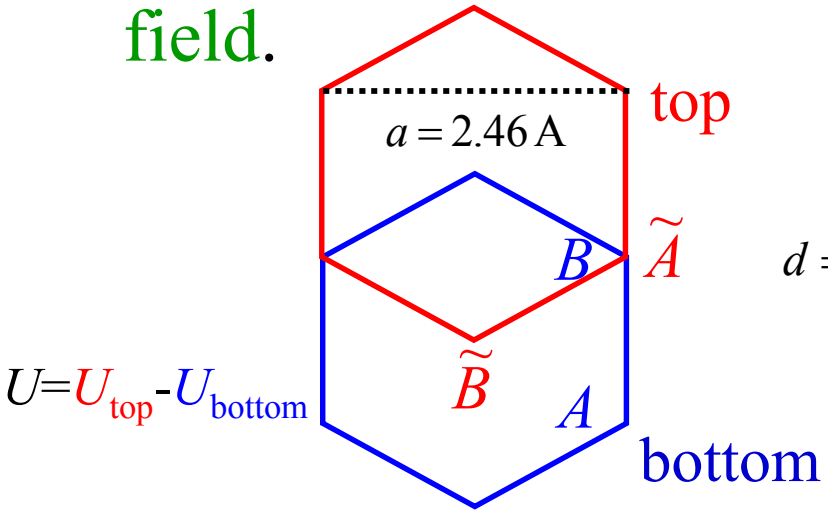


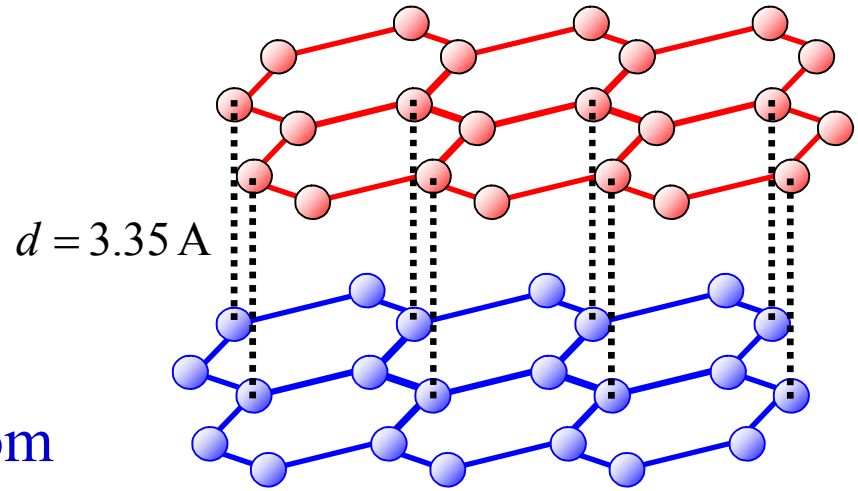


1. Introduction

2) Graphene bilayer

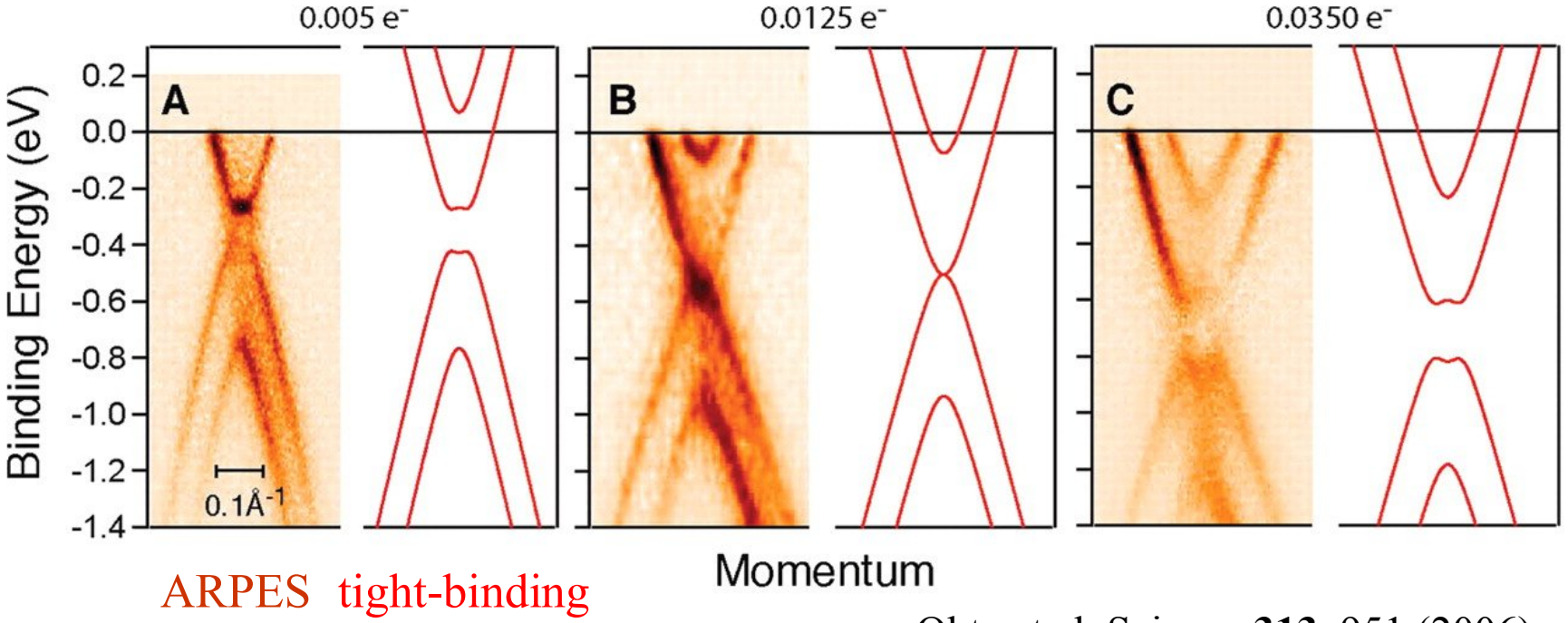
- Graphene bilayer is composed of a pair of coupled graphene monolayers.
- A band gap opens if on-site energy difference U between two layers is non-zero.
- U can be controlled by doping or an external electric field.





3) Band structure control by doping

- Angle-resolved photoemission spectroscopy (ARPES)

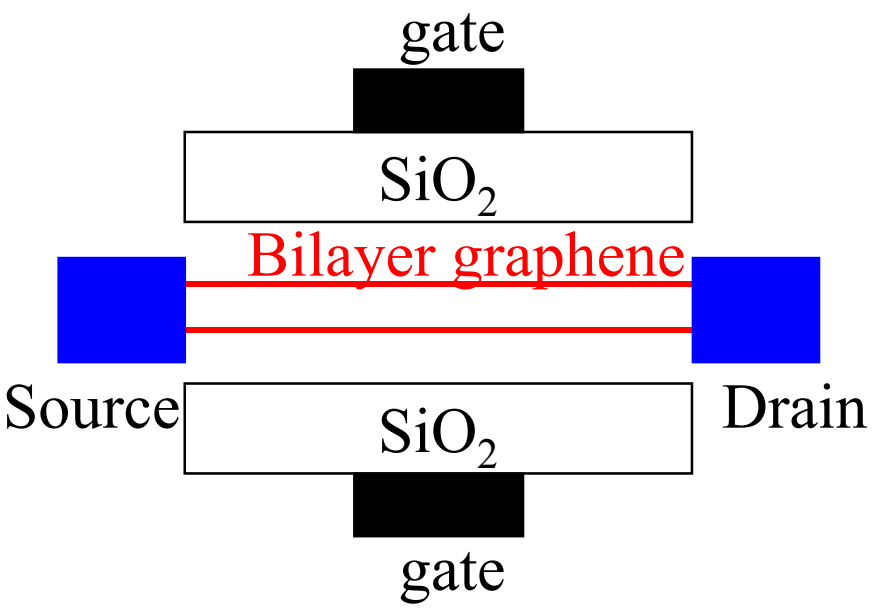


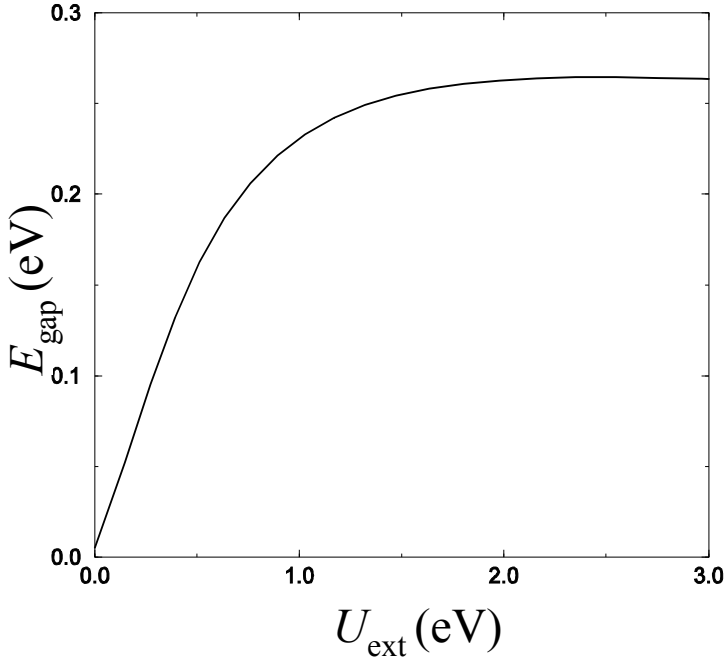
Ohta et al. Science **313**, 951 (2006)

1. Introduction

4) Band structure control by an external electric field

- Schematic illustration of a circuit with a bilayer graphene



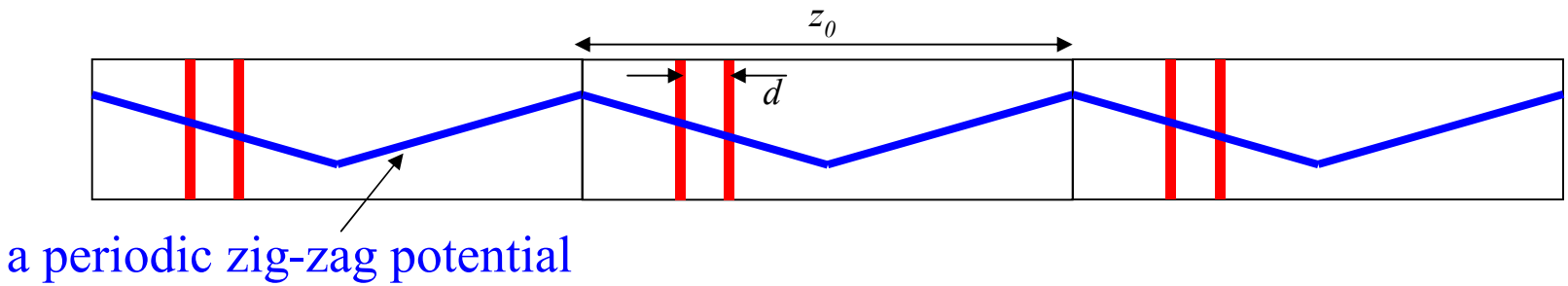


$\Rightarrow$ Possible application to a switch device

2. *Ab Initio* Calculations

1) *Ab initio* density functional theory (DFT) calculations

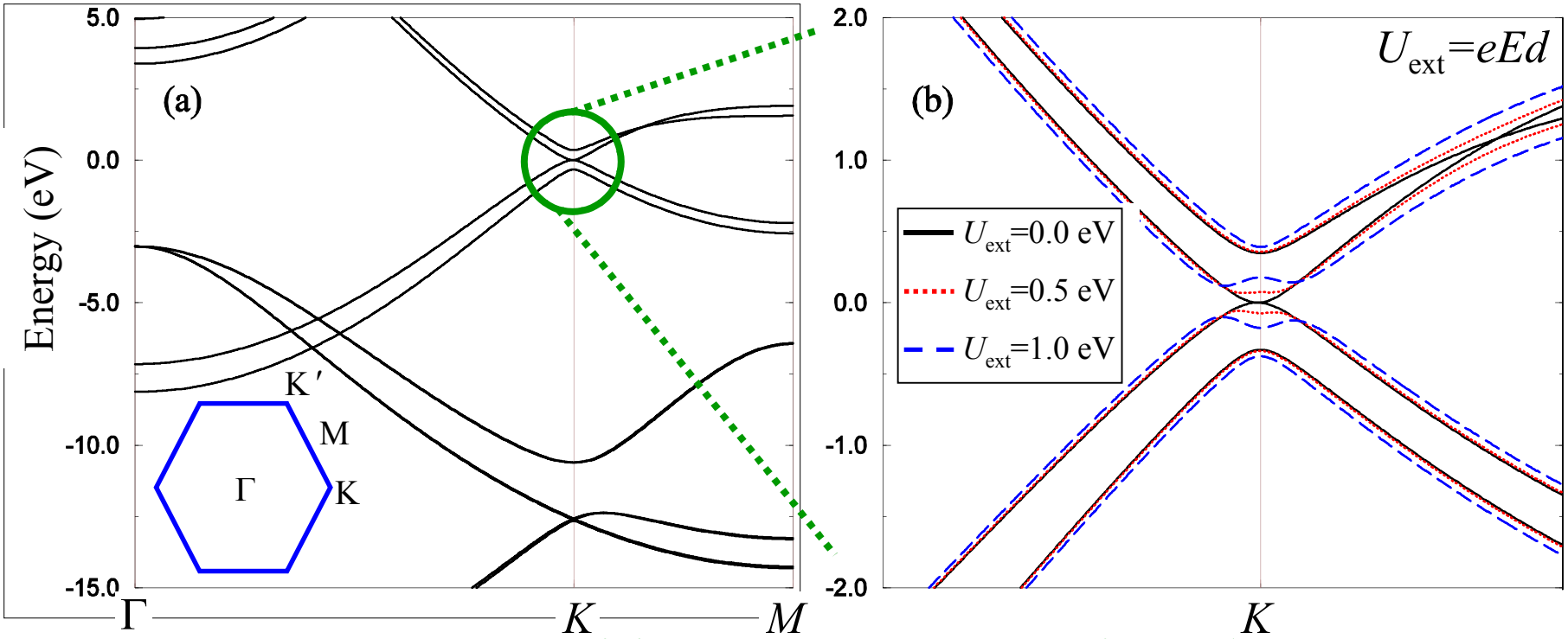
- All-electron linearized augmented plane wave
- Generalized-gradient approximation
- Supercell calculation, z_0~16A
- A periodic zig-zag potential was applied.



2. *Ab Initio* Calculations

2) Bilayer graphene band structure

- A energy gap opens by an external electric field.
- The low energy bands develop a *Mexican hat* structure.

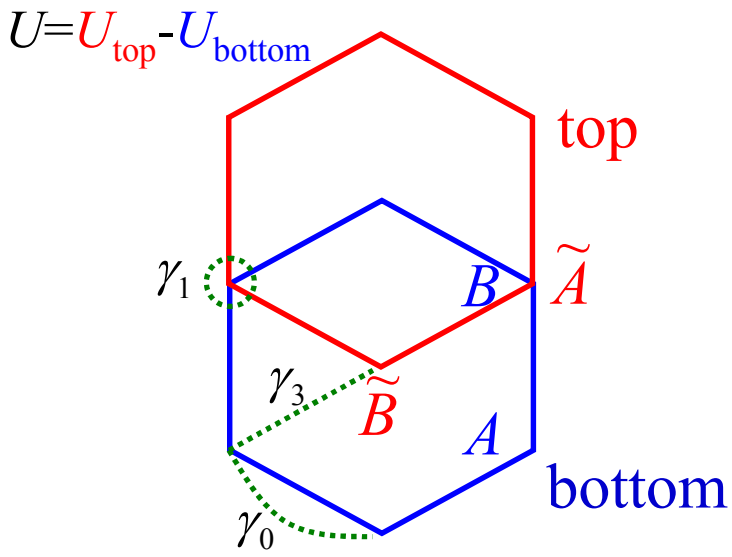


$\Rightarrow$ A tunable energy gap semiconductor

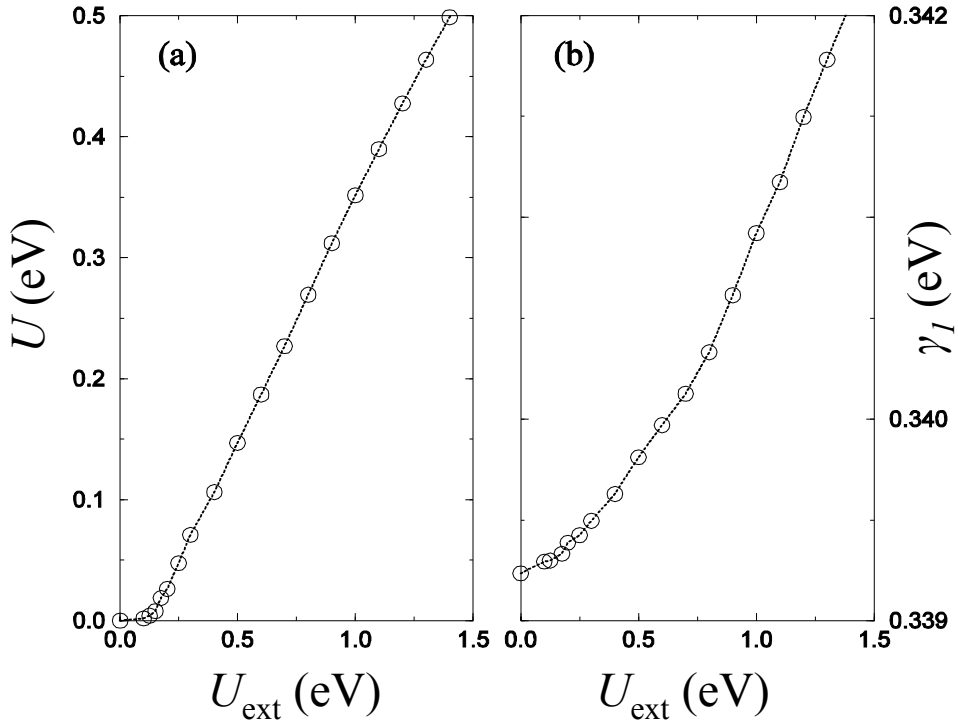
2. *Ab Initio* Calculations

3) Evolution of tight-binding parameters

- Tight-binding parameters were extracted from DFT energy bands near K.
- They show the external electric field dependence.



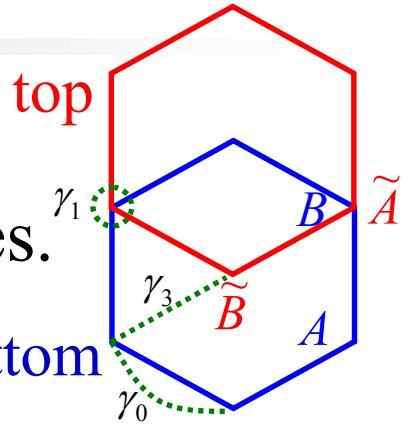
$\gamma_0 \approx 2.6\,\text{eV}, \gamma_3 \approx 0.3\,\text{eV}$

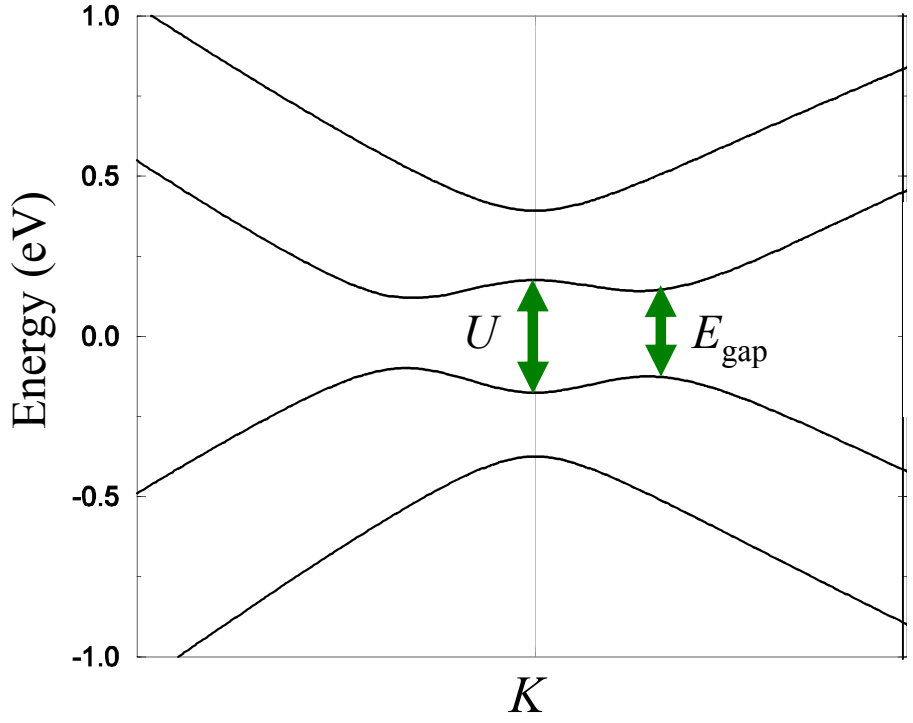


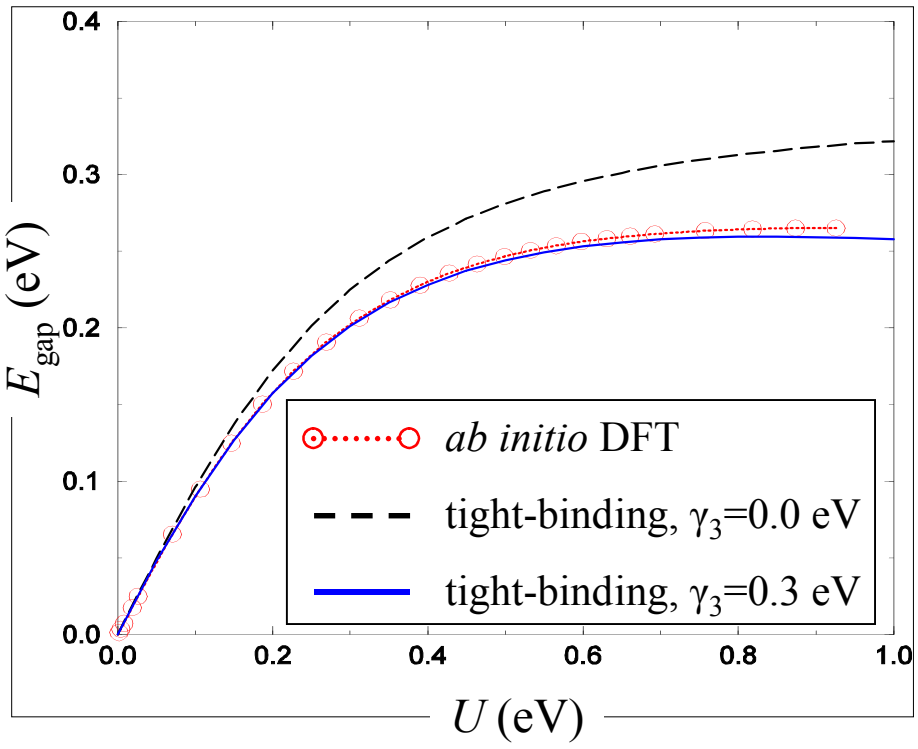
2. *Ab Initio* Calculations

4) Evolution of energy gap

- For γ_3=0, $E_{\text{gap}} = |U| r_1 / \sqrt{r_1^2 + U^2} \rightarrow r_1$ as U increases.
- Energy gap saturates ~0.3 eV.







3. Self-consistent Hartree Calculations

1) Continuum Hartree Potential Method

- A two-body interaction in a plane wave basis

$$\hat{V}=\frac{1}{2\Omega}\sum_{\mathbf{k_1},\mathbf{k}_2,\mathbf{q}}\sum_{\mu_1,\mu_2}\sum_{\sigma_1,\sigma_2}V_{\mu_1,\mu_2}(\mathbf{q})\,c^{+}_{\mathbf{k_1}+\mathbf{q},\mu_1\sigma_1}c^{+}_{\mathbf{k}_2-\mathbf{q},\mu_2\sigma_2}c_{\mathbf{k}_2,\mu_2\sigma_2}c_{\mathbf{k}_1,\mu_1\sigma_1}$$

- A mean-field Hartree approximation

$$\hat{V}^{(H)}=\sum_{\mathbf{k}}\sum_{\mu,\sigma}\varepsilon^{(H)}_{\mu}c^{+}_{\mathbf{k},\mu\sigma}c_{\mathbf{k},\mu\sigma}$$

$$\varepsilon^{(H)}_{\mu}=\frac{2}{\Omega}\sum_{\mathbf{k}}\sum_{\mu,\sigma}V_{\mu,\mu'}(0)\left\langle c^{+}_{\mathbf{k},\mu'\sigma'}c_{\mathbf{k},\mu'\sigma'}\right\rangle$$

σ	for *A, B*
μ	for top, bottom
$\mathbf{k}\in$	Brillouin zone
$\mathbf{q}\in$	whole plane

2) Lattice Hartree Potential Method

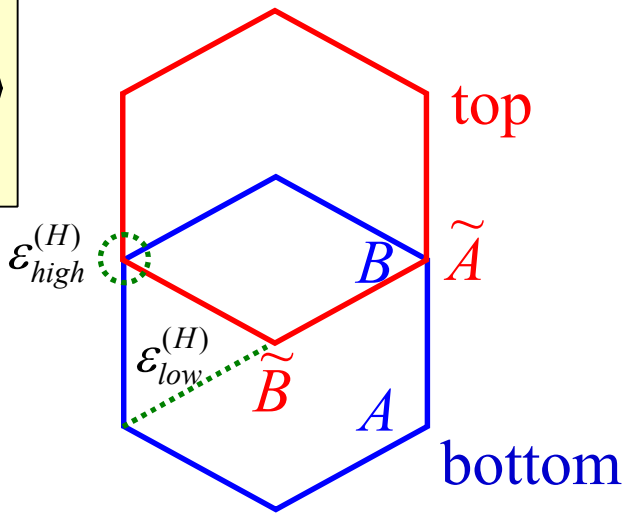
- Choose Bloch states as a basis

$$\psi_{\mathbf{k},\mu\sigma}(\mathbf{x}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \phi_{\mu\sigma}(\mathbf{x}-\mathbf{R}-\boldsymbol{\tau}_{\mu\sigma})$$

σ	for A, B
μ	for top, bottom
$\mathbf{k} \in$	Brillouin zone
$\boldsymbol{\tau}$	displacement

$$\Rightarrow \quad \varepsilon_{\mu\sigma}^{(H)} = \frac{2}{\Omega} \sum_{\mathbf{k}} \sum_{\mu,\sigma} \tilde{V}_{\mu\sigma,\mu'\sigma'}(0) \left\langle c_{\mathbf{k},\mu'\sigma'}^{+} c_{\mathbf{k},\mu'\sigma'} \right\rangle$$

$$\varepsilon_{low}^{(H)} = \varepsilon_{\tilde{B}}^{(H)} - \varepsilon_{A}^{(H)}, \quad \varepsilon_{high}^{(H)} = \varepsilon_{\tilde{A}}^{(H)} - \varepsilon_{B}^{(H)}$$

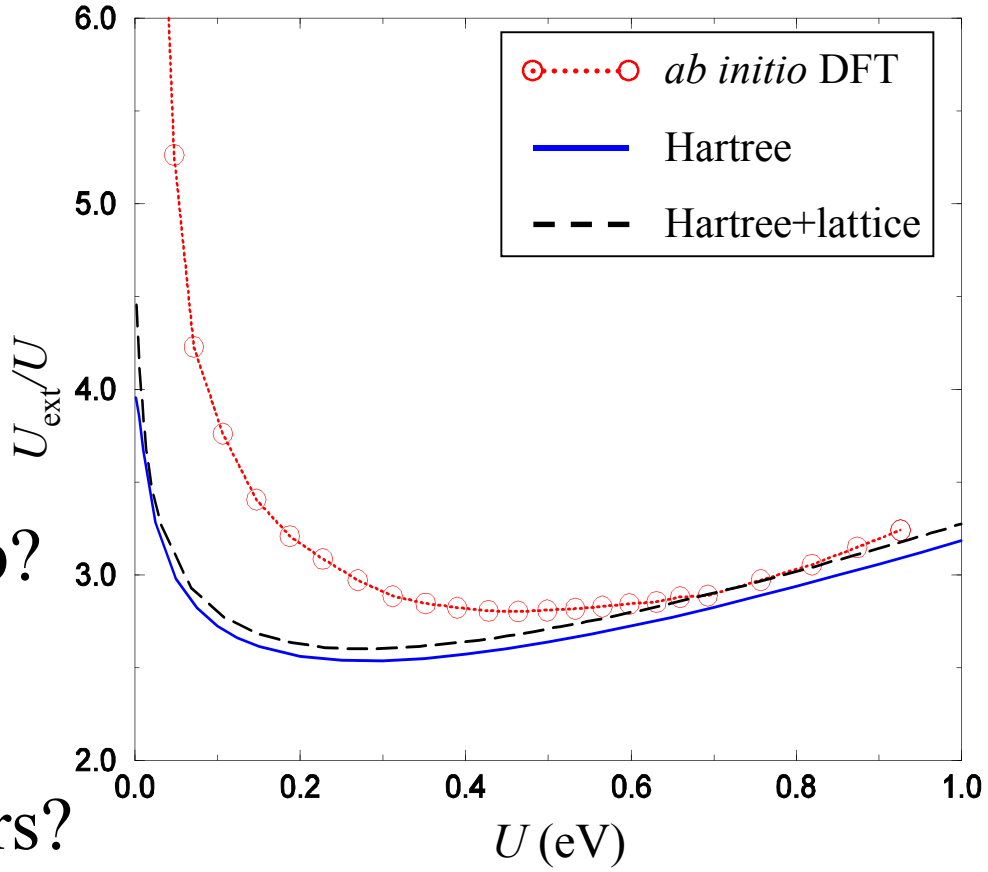


3. Self-consistent Hartree Calculations

3) Screening effects

- Enhanced screening at small U

- In DFT, the screening is more pronounced.
  - Underestimation of gap?
  - σ-orbital contribution?
  - Fitting inaccuracy in tight-binding parameters?



Summary

- Using *ab initio* density functional theory, we showed that band structure can be controlled by applying an external electric field.
- The electric field dependence of tight-binding parameters were obtained from the DFT results.
- The screening effect seen in the DFT results were compared with a tight-binding self-consistent Hartree method including crystalline inhomogeneity corrections.

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