Enhanced Many-Electron Effects in Gated Bilayer Graphene

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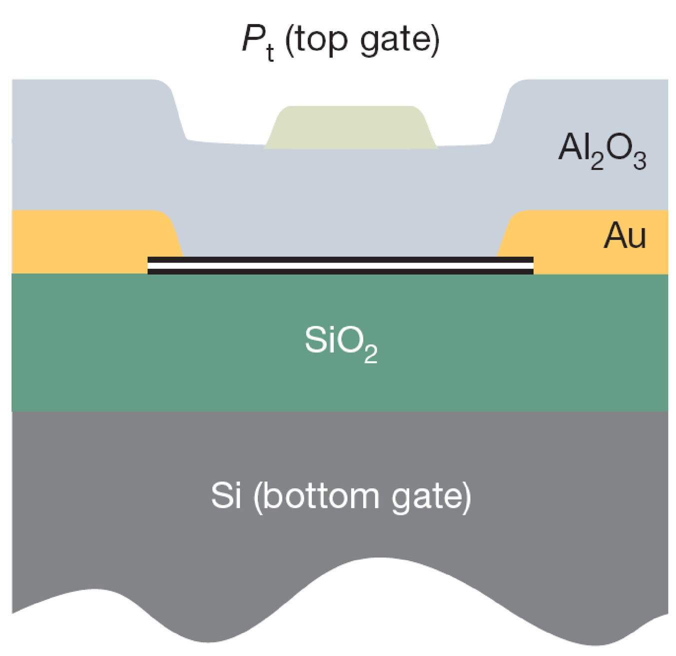
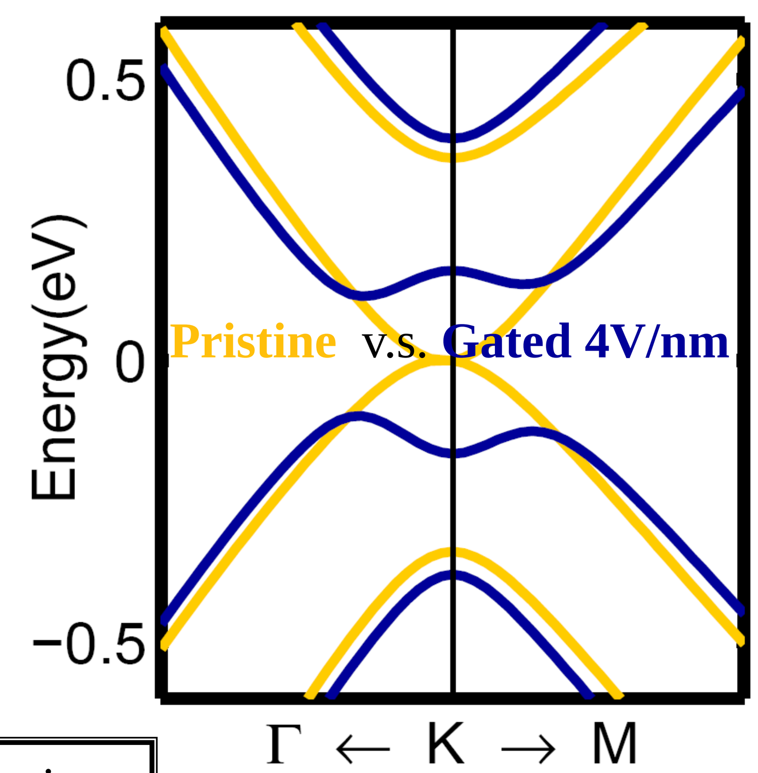
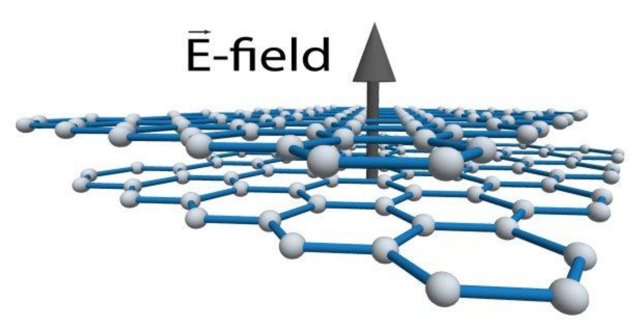
Introduction





- Gate electric field introduces band gap in bilayer graphene for bipolar and optoelectronic devices applications.**[1]**
- Unusual "Mexican-hat" band dispersion relation
- Density functional theory (DFT) underestimates band gap and no electron-hole(*e-h*) pair picture



I. Many-Body Perturbation Theory

GW-APPROXIMATION (GWA) [2]:

- Approximate self energy as the product of dressed Green's function (G) and screened Coulomb interaction (W) to calculate the Quasiparticle (QP) energies
- W: 1 / (dielectric function ε) × bare Coulomb interaction v
- Take into account electron-electron screening effects

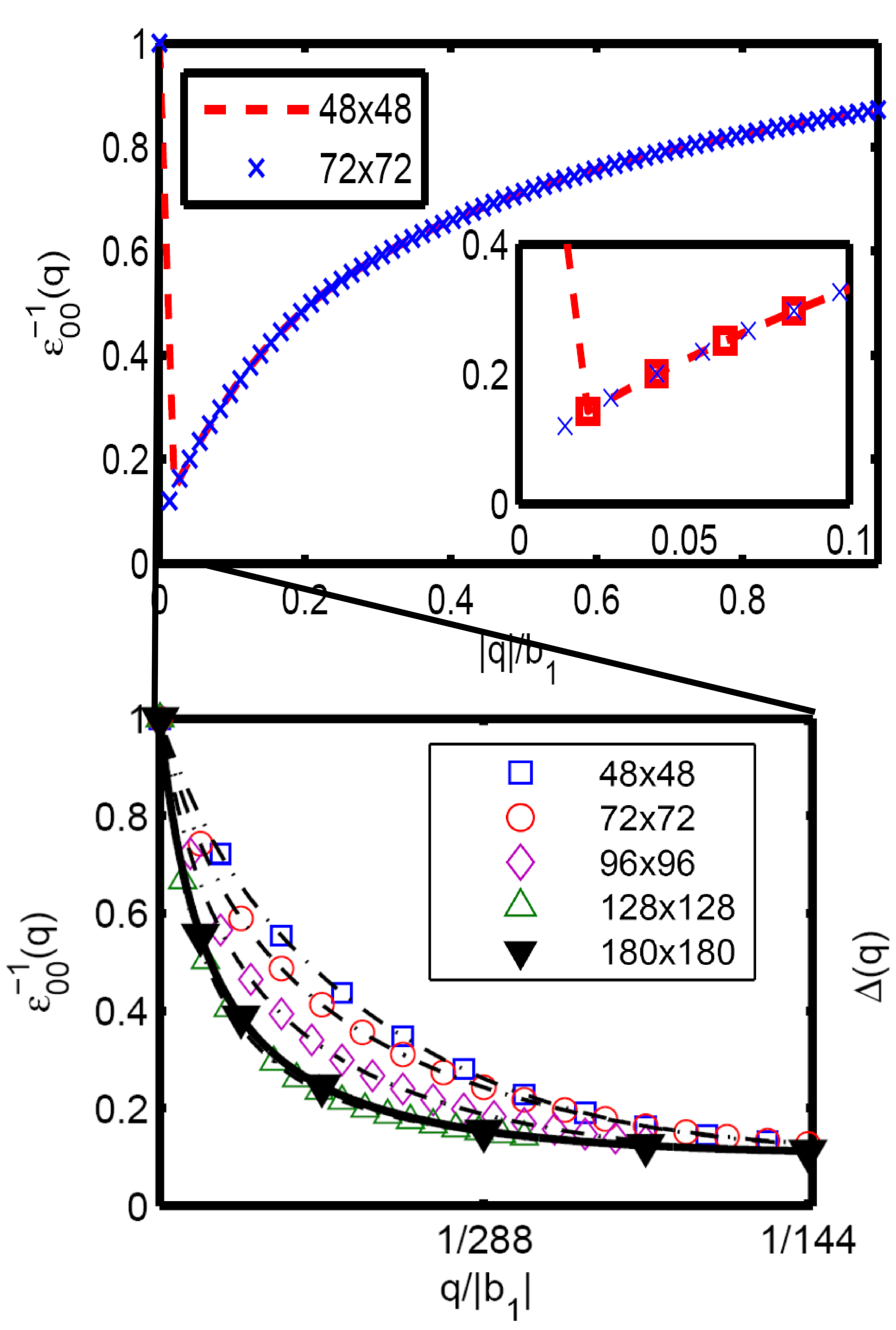
BETHE-SALPETER EQUATION (BSE) [3]:

- The *e-h* correlation is described by the BSE

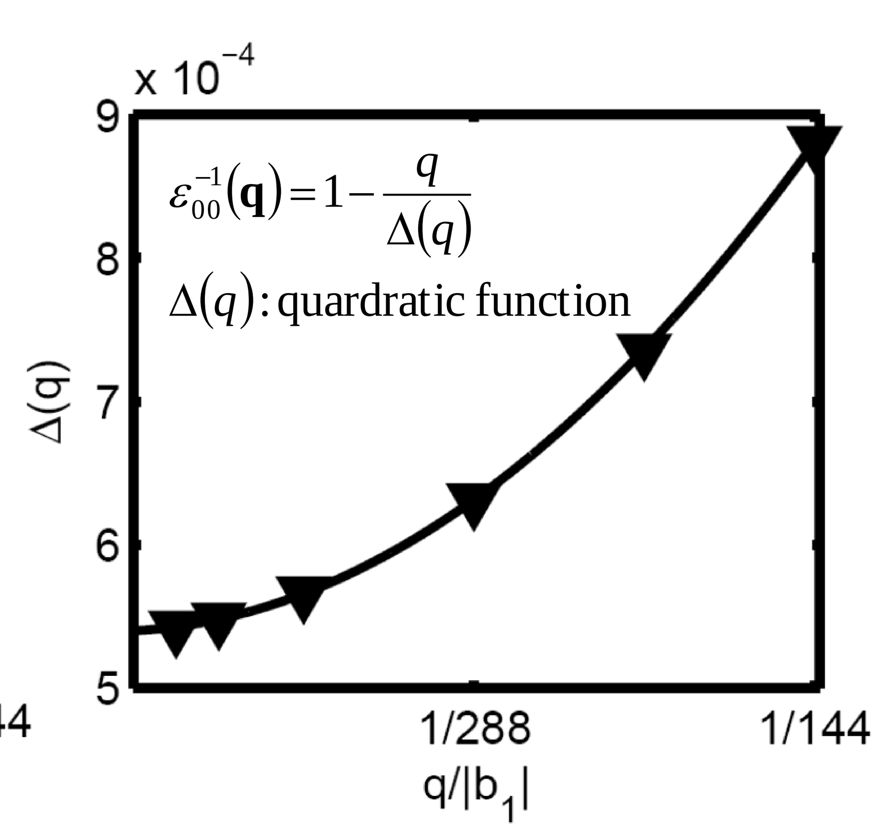
$$(E_c - E_v)A^S_{vck} + \sum_{v'c'} K^{AA}_{vck,v'c'k}(\Omega_S)A^S_{v'c'k} = \Omega_S A^S_{vck}$$

- The interaction kernel *K* depicts screened *e-h* Coulomb interaction. *Ec* and *Ev* are the previously computed QP energies .
- Give reliable *e-h* excited states that are related to the optical response of the material.

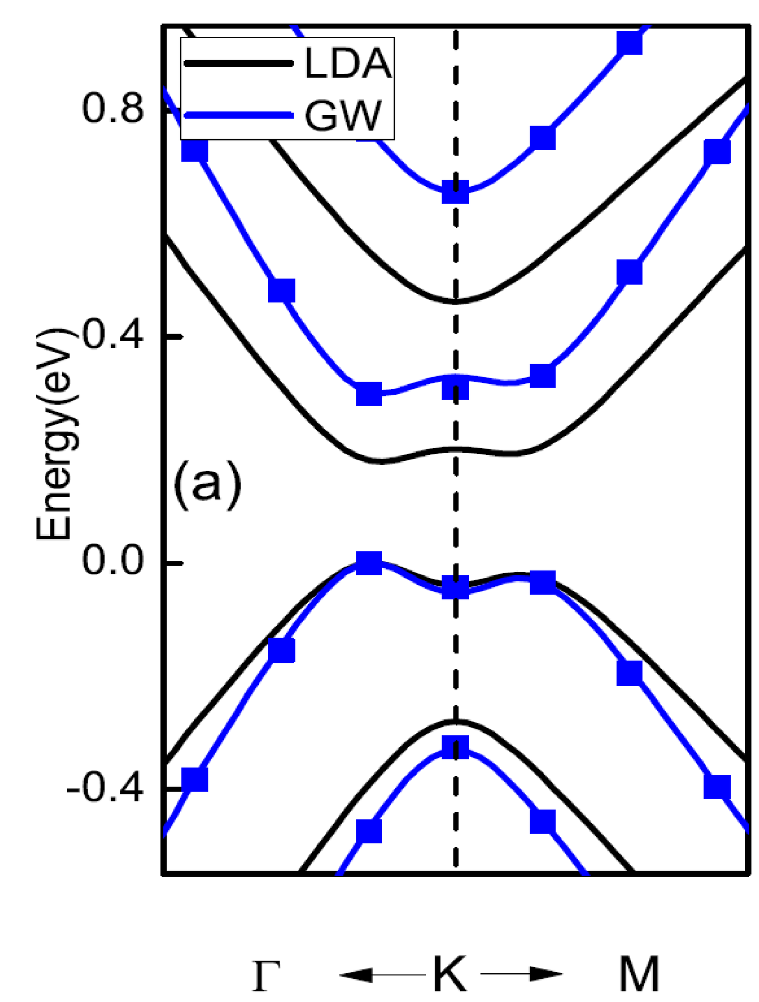
II. Modeling the Dielectric Function

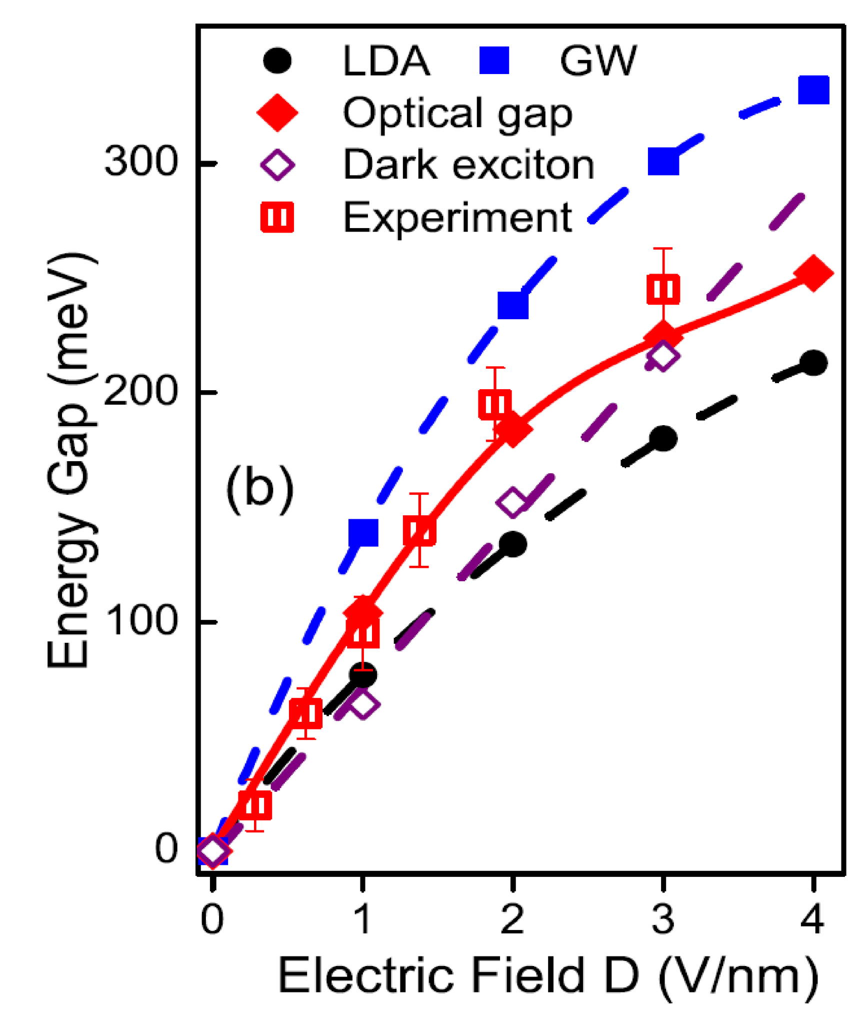


- The inverse dielectric function plays a key role in obtaining the *screened Coulomb interaction W*.
- The head component of change rapidly as q → 0
- Uniform sampling scheme is not appropriate.
- Model ε^{-1}_{00} as q → 0



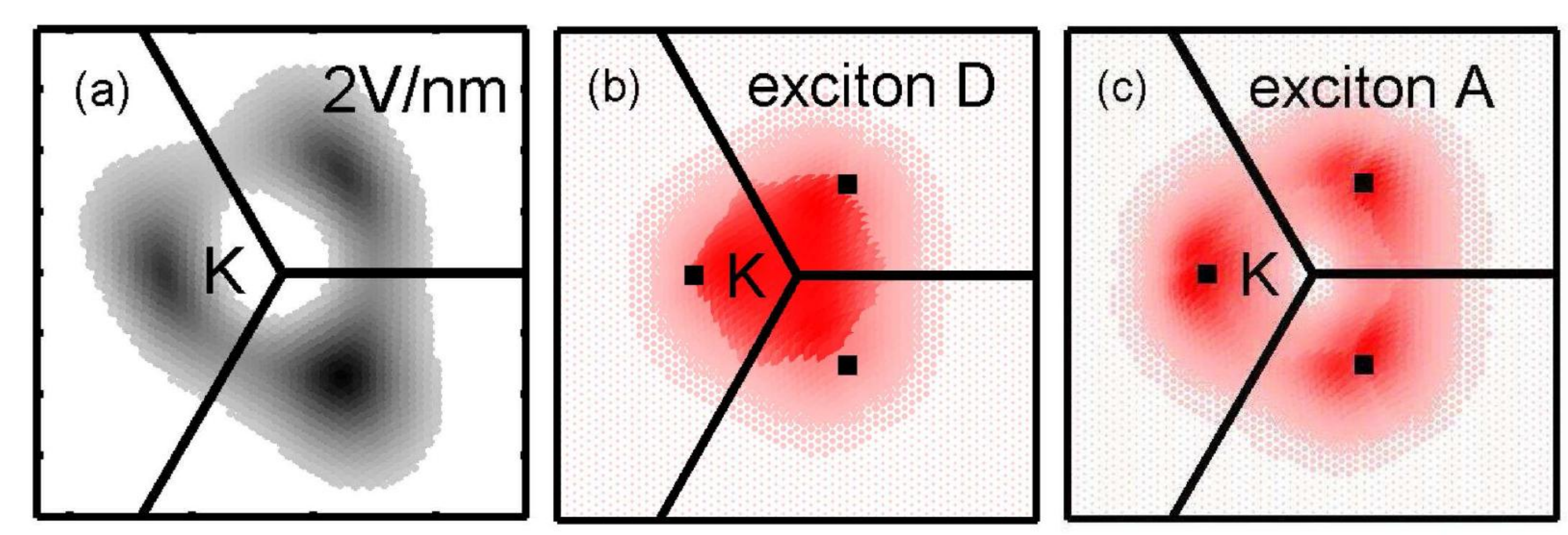
III. LDA, GW and Optical Gap



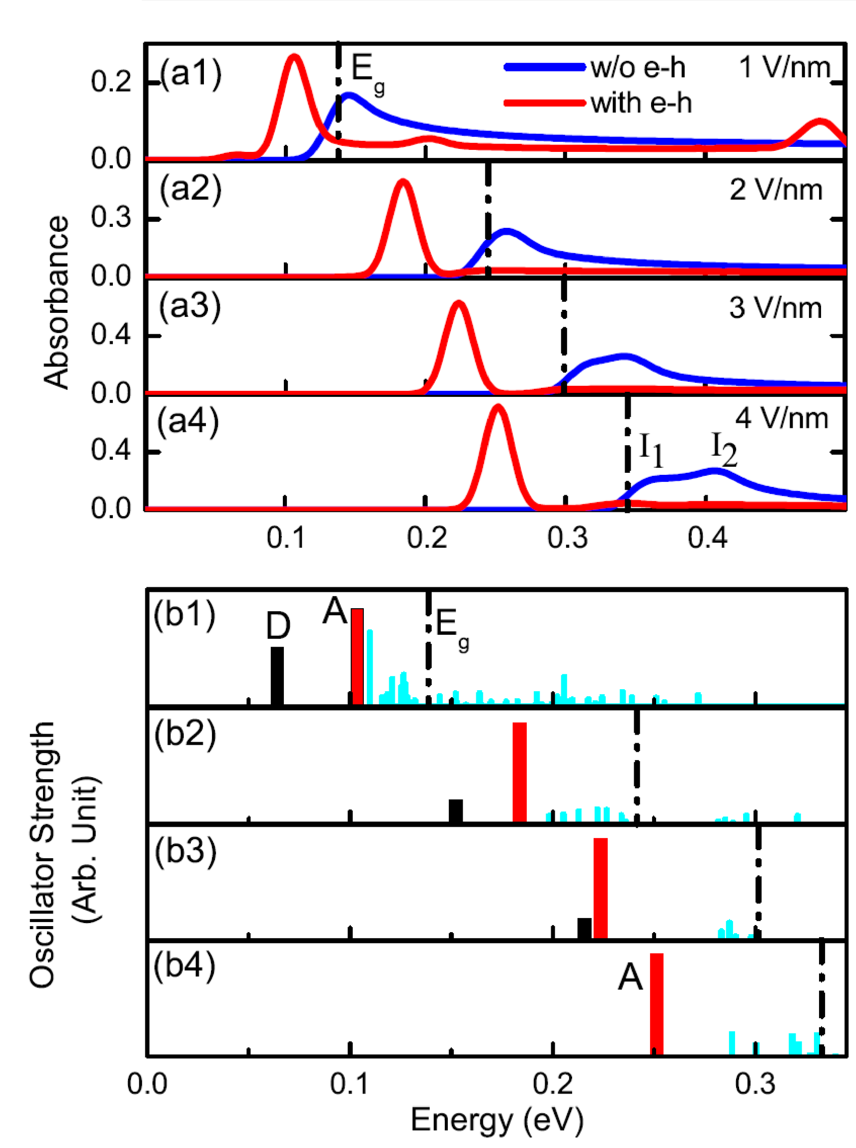


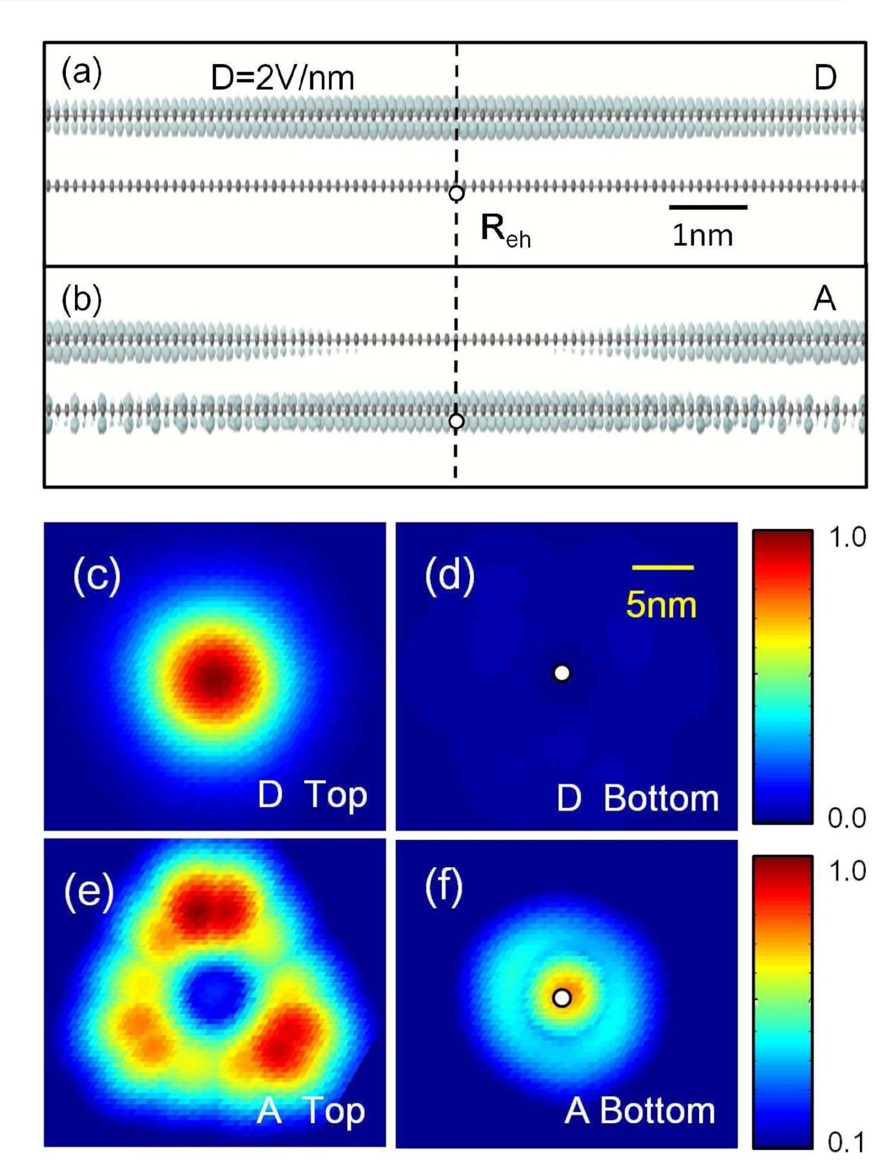
- Many-electrons effects are crucial to decide the electronic structure and optical excitations of the gated bilayer graphene (GBLG).
- Enhanced e-e interactions dramatically enlarge band gap: QP band gap by GWA > 150% of LDA band gap
- Optical gap is in excellent agreement with experiments.

IV. Excitonic Effects and Optical Absorption



(a) Single-particle transition matrix element
(b) (c) Exciton wavefunction for exciton D and A in reciprocal space





- The infrared optical absorption spectra are dictated by a bright bound excitonic state A (2-fold degeneracy)
- An unusual low-energy dark excitonic state D with *e* and *h* completely condensed into separate layers.

References and Acknowledgement

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[1] Yuanbo Zhang *et al*, Nature **459**, 820-823 (2009)
[2] Mark S. Hybertsen and Steven G. Louie, PRB **34**, 5390 (1986)
[3] Michael Rohlfing and Steven G. Louie, PRB **62**, 4927 (2000)