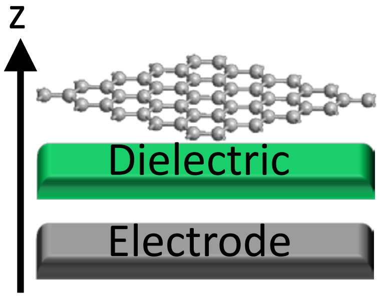
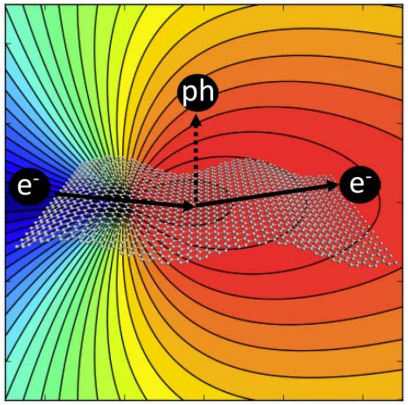
Flexural-phonon scattering induced by electrostatic gating in graphene





Graphene device – a vibrating membrane in an electrostatic and dielectric environment.
Electron-phonon coupling and mobility limitations from the environment.

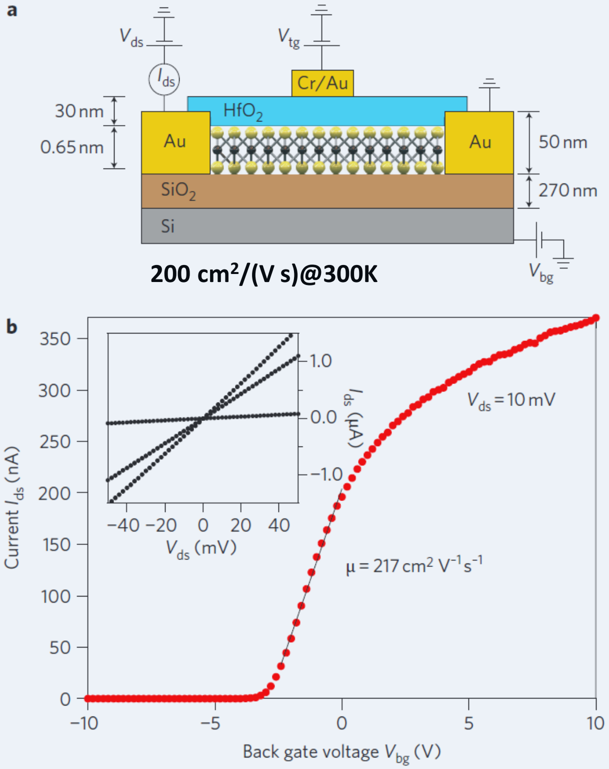
Tue Gunst,
Technical University of Denmark (DTU)

29/03-2017

Motivation – novel 2D materials and el-ph scattering

MoS$_2$ monolayer transistors

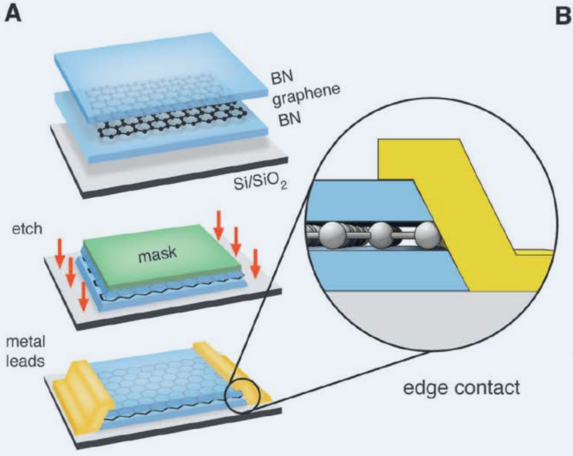
high-κ gate dielectric

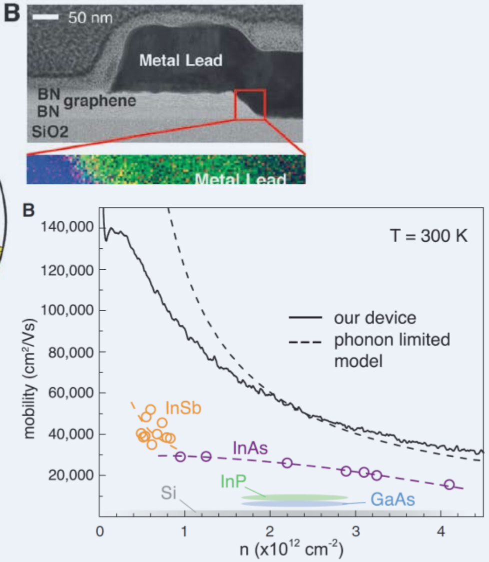


200 cm²/(V s)@300K

Single-layer MoS2 transistors
B. Radisavljevic *et al.*, Nature Nanotechnology, VOL 6 (2011)

Graphene monolayer transistors



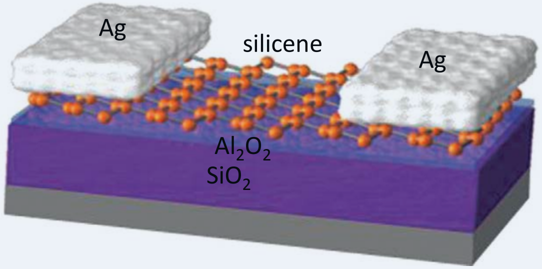


90.000 cm²/(V s)@300K and 1 10¹²/cm².
45.000 cm²/(V s)@300K and 3 10¹²/cm².

One-Dimensional Electrical Contact to
a Two-Dimensional Material
L. Wang *et al.*, Science, VOL 342 (2013)

Encapsulation, edge contacting
suspend in high-κ liquid->
screen charged impurities

Silicene monolayer transistors

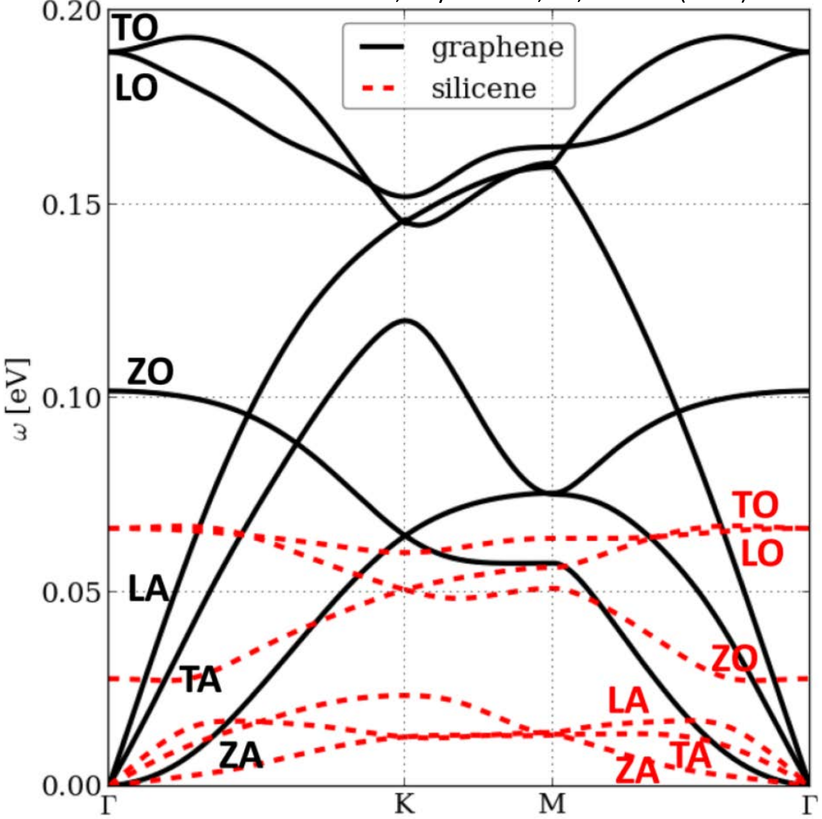


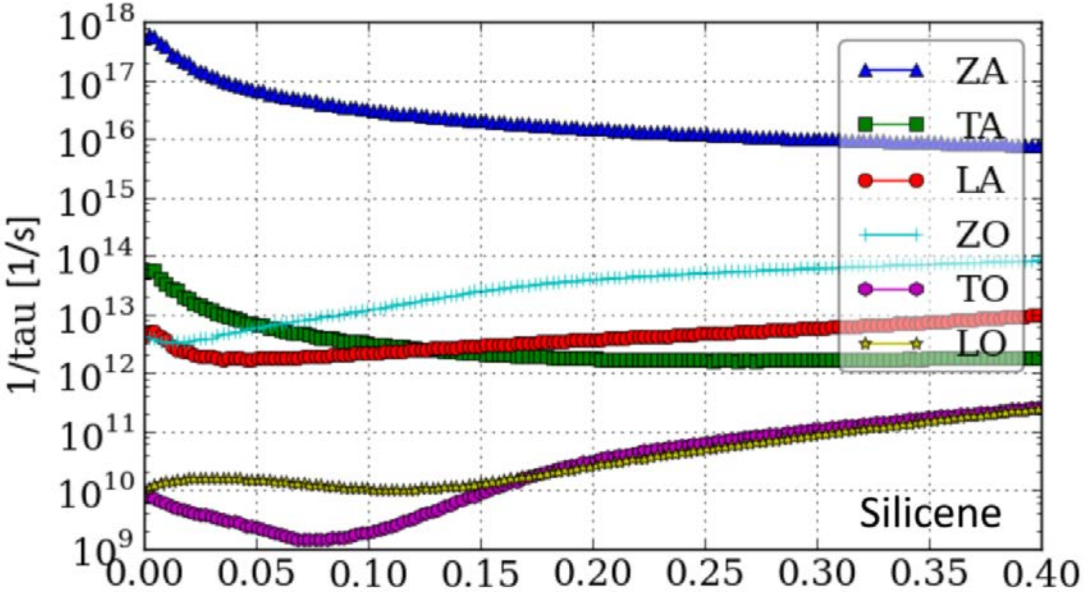
Grown at Ag+flip+pattern
100 cm²/(V s)@300K

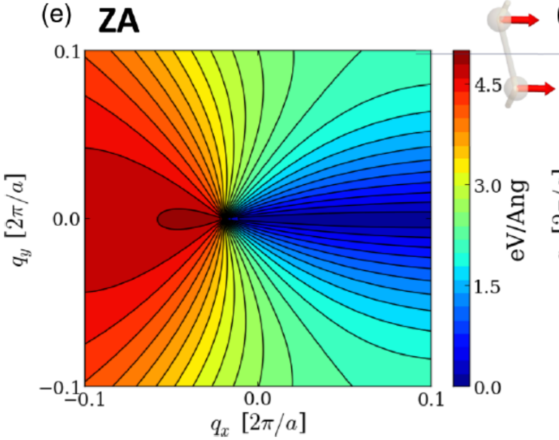
Silicene field-effect transistors operating
at room temperature
Li Tao *et al.*, Nature Nanotechnology, VOL 10 (2015)

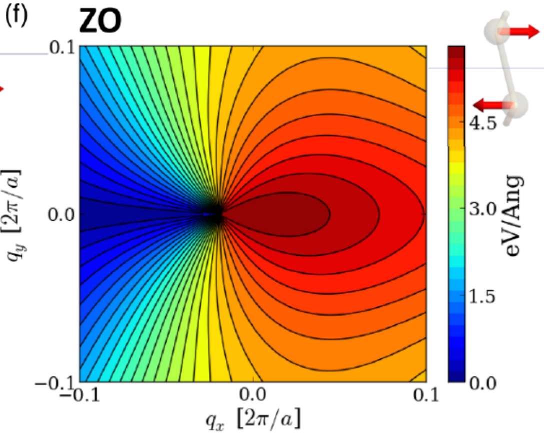
Motivation – Silicene (a 2D material with broken planar mirror symmetry)

T. Gunst *et al.*, Phys. Rev. B, **93**, 035414 (2016).









ZA: Flexural membrane mode with quadratic dispersion

$\mu_e \approx 10$ cm^2/Vs (T = 300K and carrier density = 3×10^{12} cm^{-2}).

Silicon $\mu_e \approx 1400$ cm^2/Vs

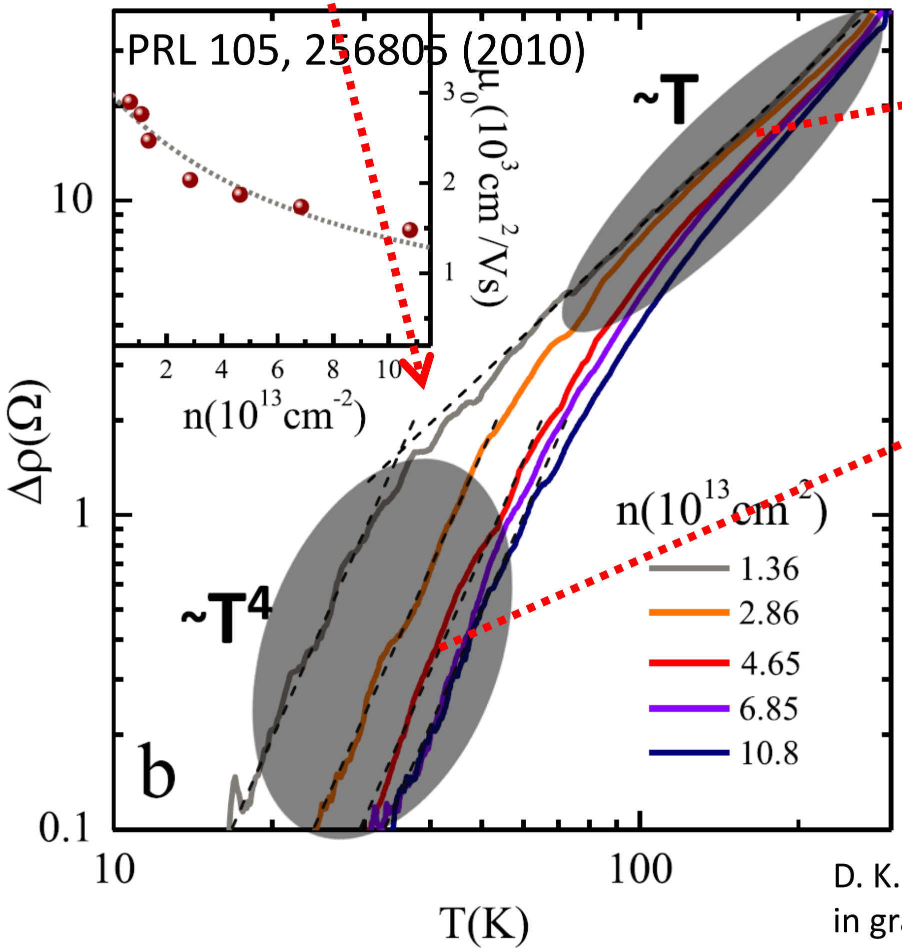
Putting graphene in a gated device stack can also break the planar mirror symmetry!

Temperature regimes

T << T_{BG}: phonon system is degenerate [Bloch-Grüneisen (BG)]
T >> T_{BG}: phonon system is nondegenerate [equipartition (EP)].

$$T_{\text{BG}} = \quad 2v_{\text{ph}}k_F/k_B \approx 54\sqrt{n}\ \text{K}$$

With n in units of $n = 10^{12}\ \text{cm}^{-2}$

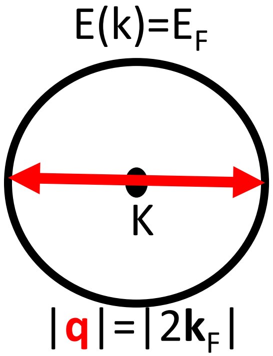


EP-regime:

$$n_B(\omega_q) \approx \frac{k_B T}{\hbar\omega_q}$$

BG regime:
Backscattering

$$k_B T_{BG} = 2k_F v_s$$



T dependence -> details of phonons (flexural, substrate interaction) and impurities.

D. K. Efetov and P. Kim, "Controlling electron-phonon interactions in graphene at ultrahigh carrier densities," PRL 105, 256805 (2010)

Summary of semiclassical BTE method

Phonon scattering rates (from k to k') – absorption/emission of a phonon (FGR):

$$P_{\mathbf{kk'}}^{\lambda nn'} = \frac{2\pi}{\hbar}|g_{\mathbf{kk'}}^{\lambda nn'}|^2\Big[n_{\mathbf{q}}^{\lambda}\delta\left(\epsilon_{\mathbf{k'}n'} - \epsilon_{\mathbf{k}n} - \hbar\omega_{q\lambda}\right)\delta_{\mathbf{k'},\mathbf{k+q}} + (n_{-\mathbf{q}}^{\lambda} + 1)\delta\left(\epsilon_{\mathbf{k'}n'} - \epsilon_{\mathbf{k}n} + \hbar\omega_{-q\lambda}\right)\delta_{\mathbf{k'},\mathbf{k-q}}\Big]$$

Transport relaxation time:

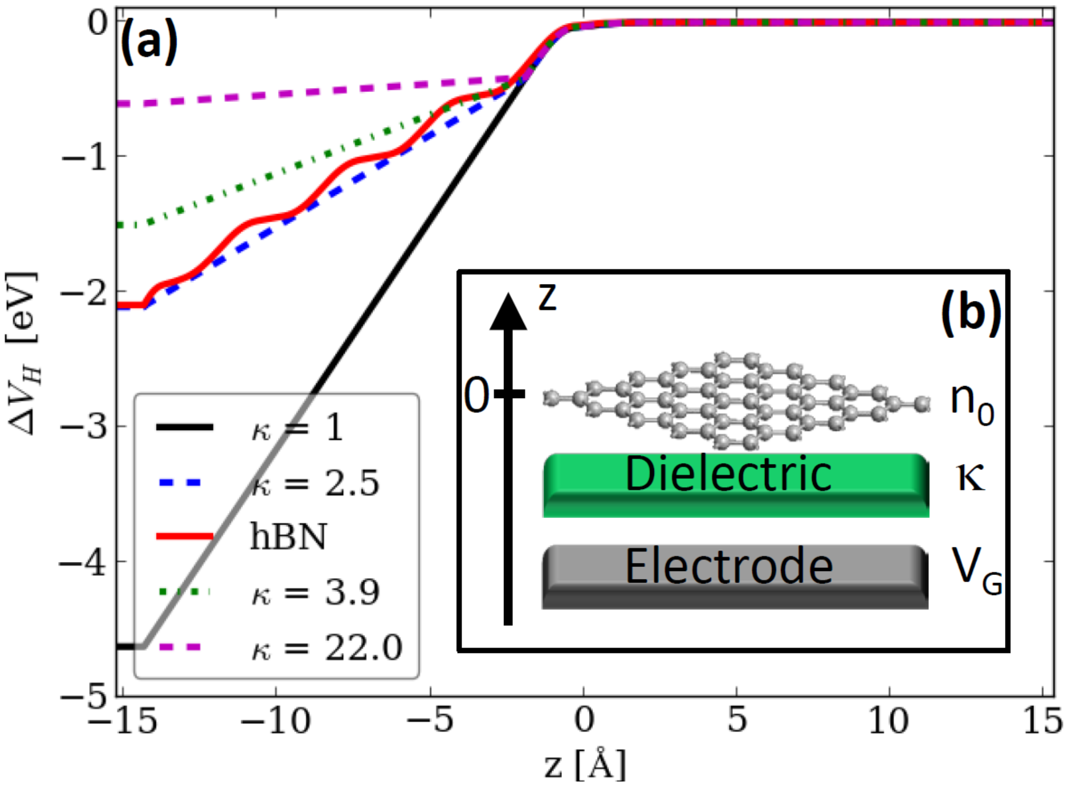
$$\boxed{\frac{1}{\tau_{\mathbf{k}n}} = \sum_{\mathbf{k'}n'}\frac{(1 - f_{\mathbf{k'}n'}^{0})}{(1 - f_{\mathbf{k}n}^{0})}\left(1 - \cos(\theta_{\mathbf{kk'}})\right)P_{\mathbf{kk'}}^{nn'}}\quad , \quad \cos(\theta_{\mathbf{kk'}}) = \frac{\mathbf{v}_{\mathbf{k'}\mathrm{n'}}\cdot\mathbf{v}_{\mathbf{k}\mathrm{n}}}{|\mathbf{v}_{\mathbf{k'}\mathrm{n'}}||\mathbf{v}_{\mathbf{k}\mathrm{n}}|}$$

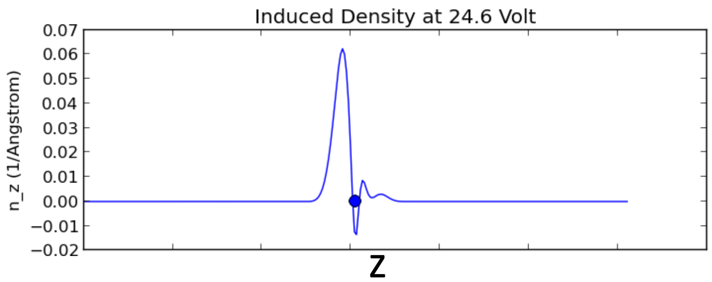
Mobility:

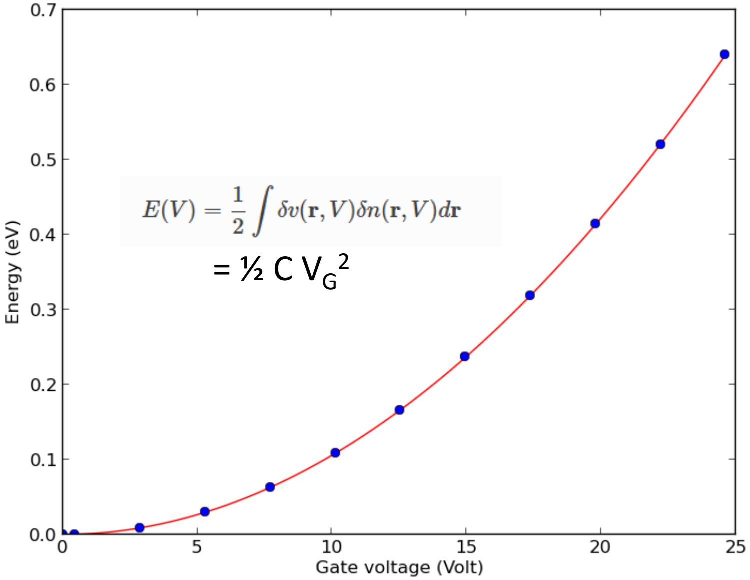
$$\mu_e = -2q\frac{\sum_{\mathbf{k}n\in c}|\mathbf{v}_{\mathbf{k}n}|^2\frac{\partial f_{\mathbf{k}n}^{0}}{\partial\epsilon_{\mathbf{k}n}}\tau_{\mathbf{k}n}}{\sum_{\mathbf{k}n\in c}f_{\mathbf{k}n}^{0}}$$

T. Gunst, T. Markussen, K. Stokbro, M. Brandbyge, "First-principles method for electron-phonon coupling and electron mobility: Applications to 2D materials", Phys. Rev. B, **93**, 035414 (2016).

A graphene capacitor







$$E(V) = \frac{1}{2}\int \delta v(\mathbf{r},V)\delta n(\mathbf{r},V)d\mathbf{r}$$

$$= \tfrac{1}{2}\, C\, V_G^2$$

$$\mathcal{E} = \frac{V_G}{d} = \frac{e n_0}{\kappa \epsilon_0}$$

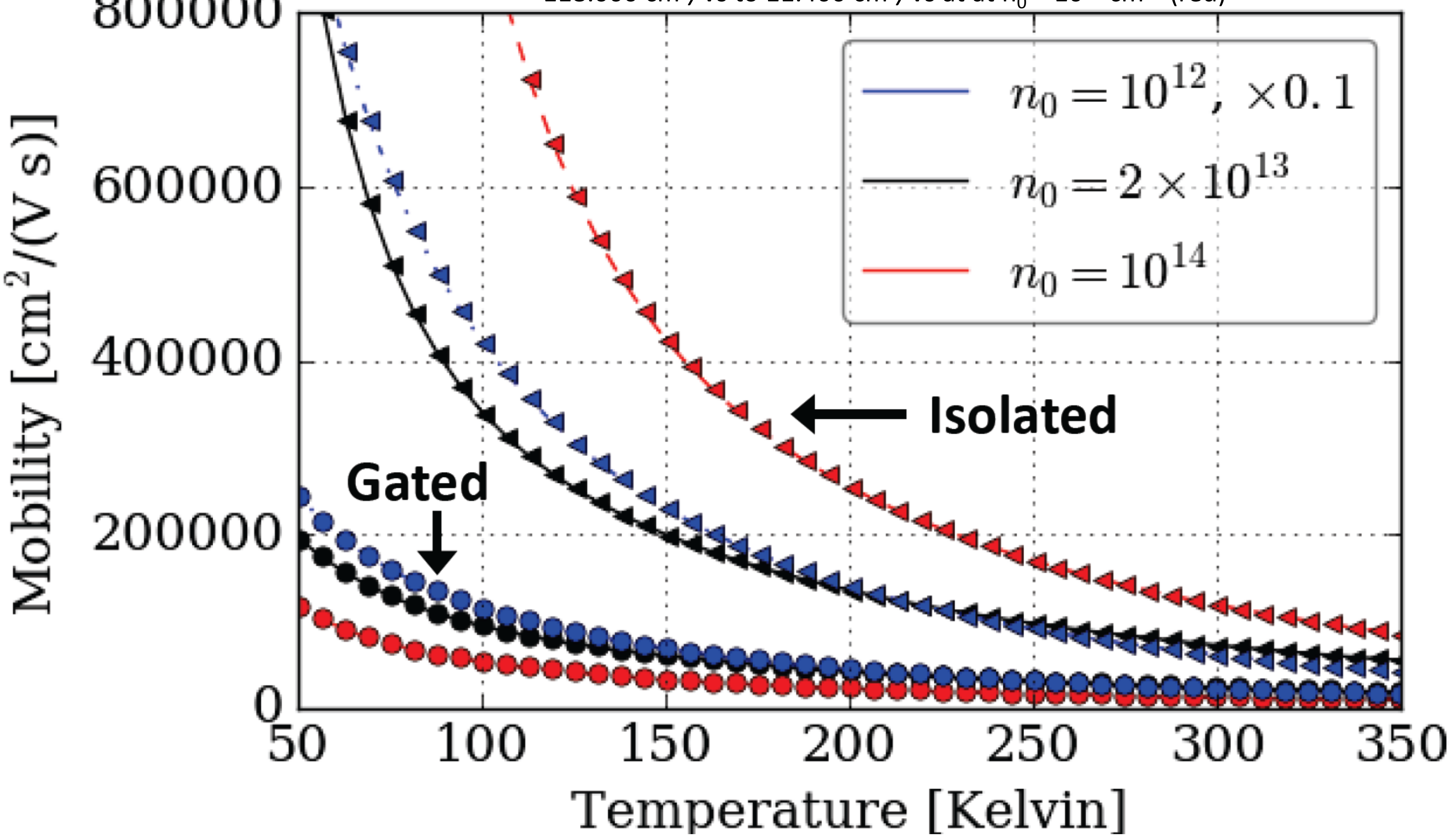
Highly doped graphene is efficient in screening the potential.
Behaves much like a metal-plate capacitor.
Gate field breaks planar mirror symmetry!

Mobility degradation

300K:

606.000 cm²/Vs to 208.500 cm²/Vs at $n_0 = 10^{12}$ cm^{-2} (blue; scaled by 0.1)

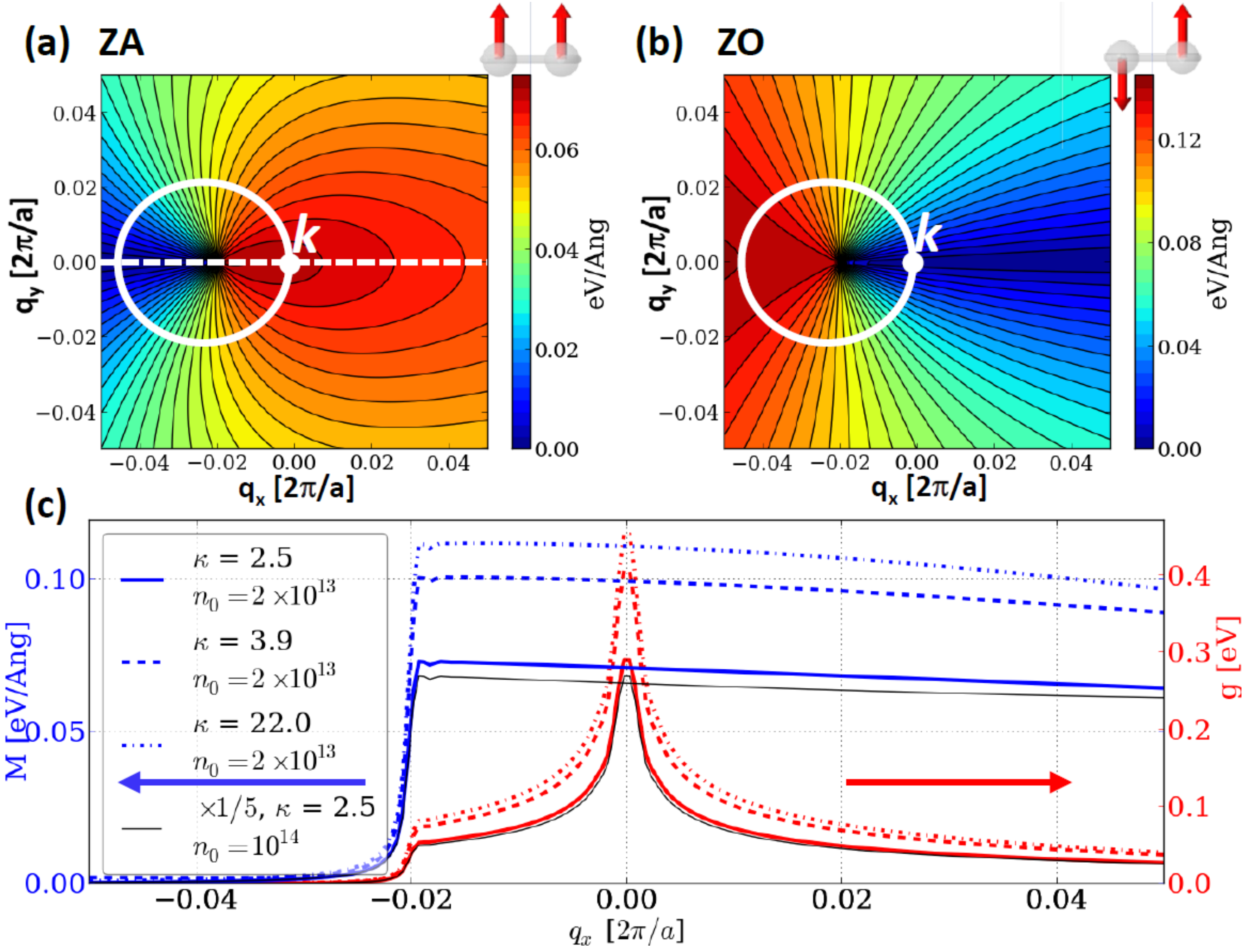
118.000 cm²/Vs to 11.400 cm²/Vs at at $n_0 = 10^{14}$ cm^{-2} (red)



Significant (field-induced) degradation!

Modified scaling with temperature and carrier density!

Ingredients - Field-induced flexural scattering



Field-induced DP:

$$D_0(V_G) \equiv \gamma n_0$$

$\gamma = 35\ (55)$ eV·Å

for $\kappa = 2.5\ (22)$

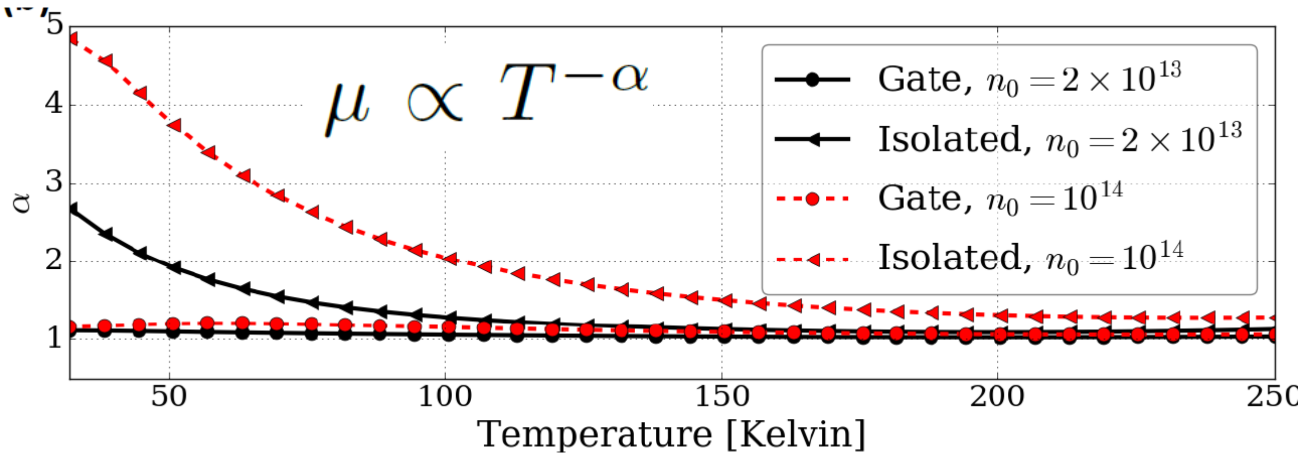
High occupation of (low frequency, constant DOS) ZA mode.

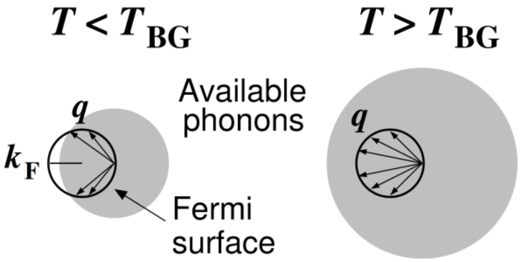
Nonzero coupling induced by the gate.

Coupling is linear in the induced carrier density and increases with dielectric constant.

Temperature scaling

Dirac model: $$\frac{1}{\tau_k^{ZA}} = \frac{v_F D_0^2(V_G)}{2\pi\rho b^2}\varepsilon_k^{-2}\frac{k_B T}{q_c}$$





BG regime:

$$q_{\max} = 2k_F$$

$$k_B T_{\mathrm{BG}} = \hbar\omega_{q_{\max}}$$

$$T_{\mathrm{BG}}^{\mathrm{LA}} = 57\sqrt{\tilde{n}}\,\mathrm{K}$$

$$T_{\mathrm{BG}}^{\mathrm{ZA}} = 0.46\,\tilde{n}\,\mathrm{K}$$

$$\tilde{n} = n/10^{12}\ \mathrm{cm}^{-2}$$

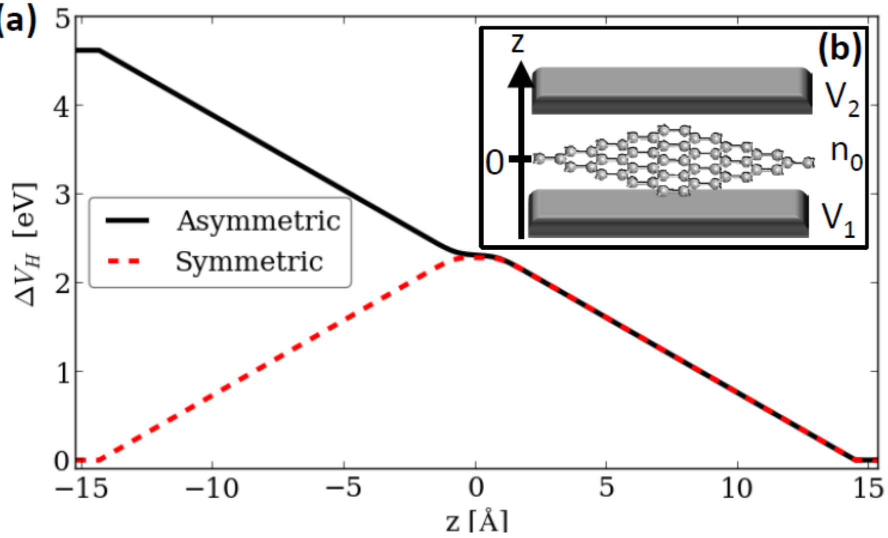
Dominant mechanism at room temperature and even more at low T!

Modified scaling with temperature!

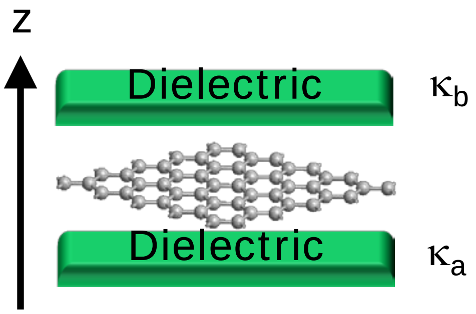
Room T: Indistinguishable from in-plane scattering (Higher DP).

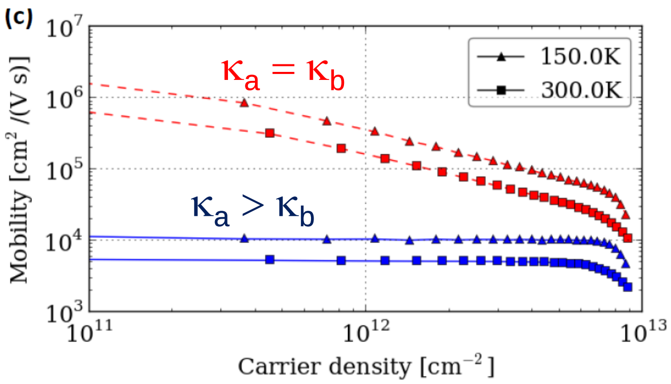
Electrode configuration – controlling the effect

Double gate stack



Dielectric sandwich





Breaking the symmetry or not?
Sandwiching graphene between two layers with different dielectric constants or electrodes at different potentials degrades mobility significantly.

Experimental signatures

Modified carrier density scaling:

$$\mu \sim n_0^{-3/2} \quad \text{Vs.} \quad \mu \sim 1/n_0 \ (\sqrt{n_0})$$

When gate-induced flexural scattering dominates.

Modified temperature scaling:

$$\mu \propto T^{-\alpha}$$

α=1 Vs. $1 < \alpha \lesssim 5$

When gate-induced flexural scattering dominates transport in the in-plane BG regime.

T< $T_{\mathrm{BG}} \approx 57\sqrt{\tilde{n}}\ \mathrm{K}$ $\quad \tilde{n} = n/10^{12}\ \mathrm{cm}^{-2}$

Gating strategy:

Double gate setup can be utilized to turn the effect on and off by generating a symmetric or asymmetric potential across the device.

Conclusions:

- New “Field induced flexural-phonon” scattering mechanism defines a relation between device symmetry and resulting mobility.
- Protecting the planar mirror symmetry is of utmost importance to fully exploit the unique transport properties of graphene.

T. Gunst, K. Kaasbjerg, M. Brandbyge, “Flexural-phonon scattering induced by electrostatic gating in graphene”, Physical Review Letters, **118**, 046601 (2017).
T. Gunst, T. Markussen, K. Stokbro, M. Brandbyge, “First-principles method for electron-phonon coupling and electron mobility: Applications to 2D materials”, Phys. Rev. B, **93**, 035414 (2016).