

# Photo-induced structural changes in graphene multilayers

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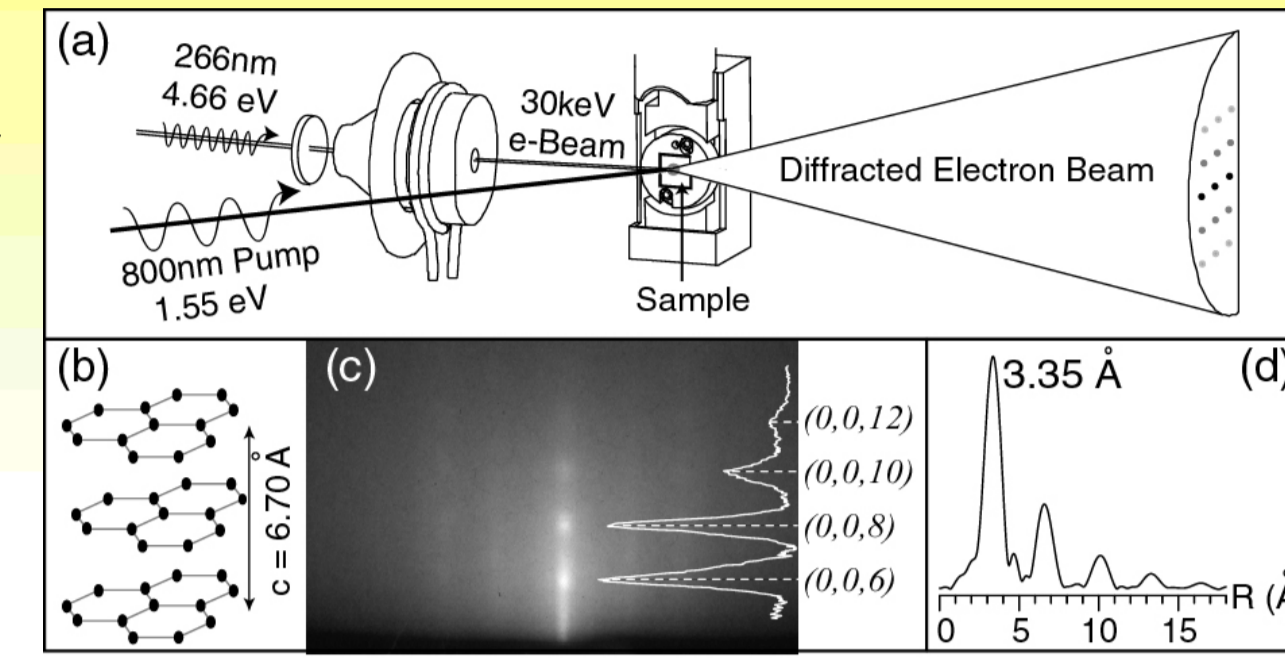
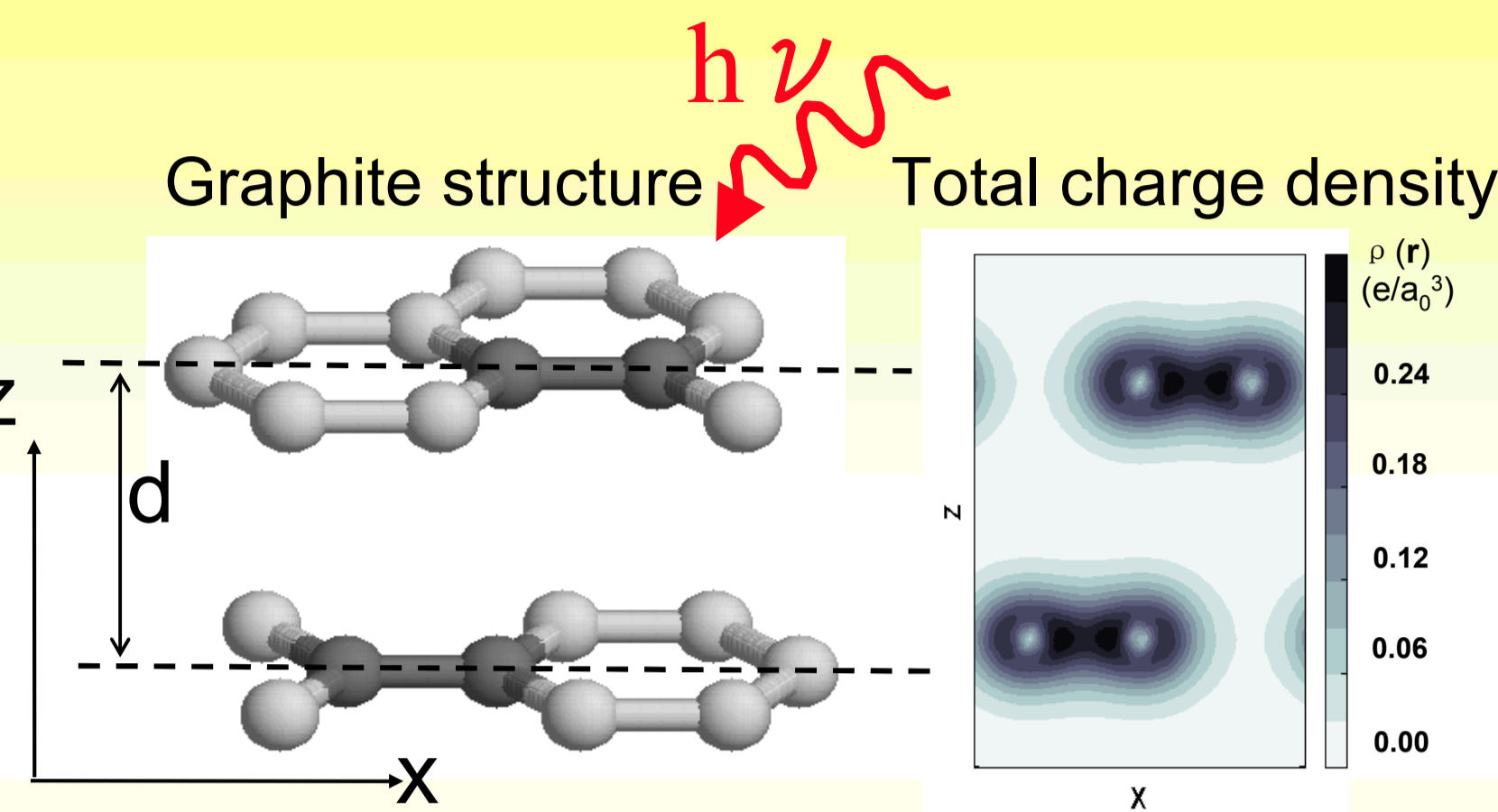
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## Our aim

Change of graphite structure by photo-excitation

(Why should it change?)

DFT simulation on photo-induced structural change

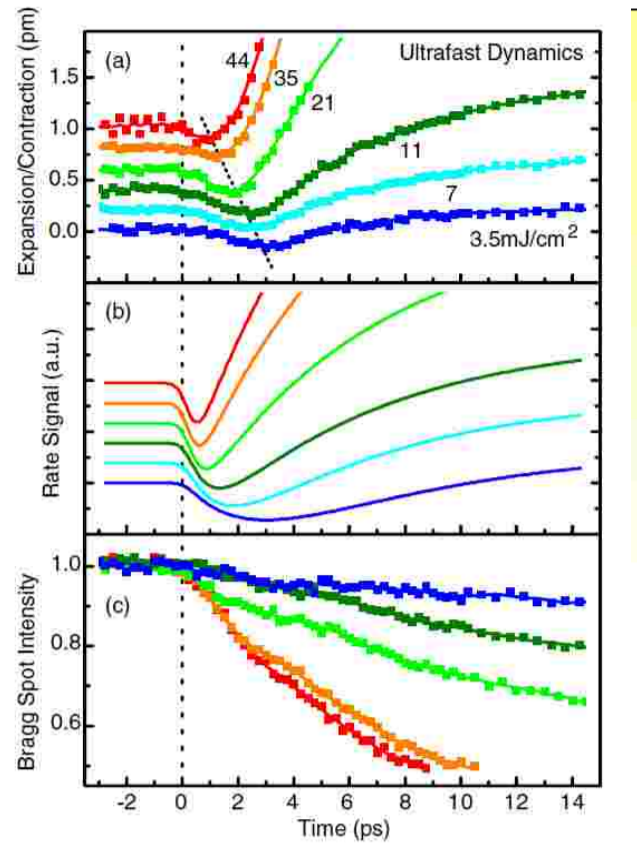


Experiment at MSU  
Time-resolved electron diffraction following laser pulse (Prof. Ruan's Gr)

Experiment at Prof. Zewail's group:

Early contraction and later expansion of inter-layer distances.

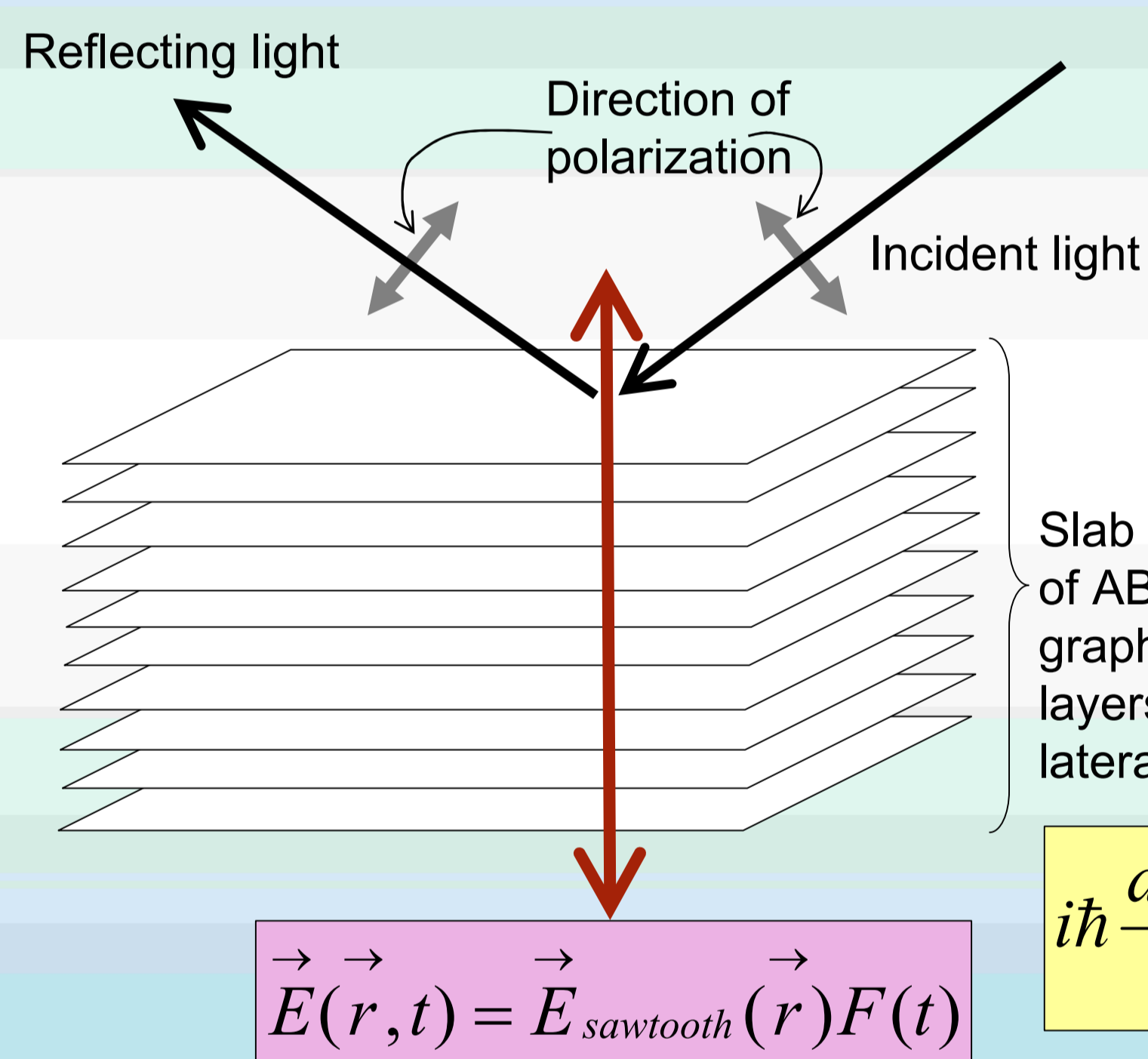
F. Carbone et al., PRL 100, 035501 (2008).



Sub-pico second: Electron-ion dynamics under pulse shot

Over pico second: MD under promoted occupation of electrons

## Sub-pico second dynamics (TDDFT-MD simulation)

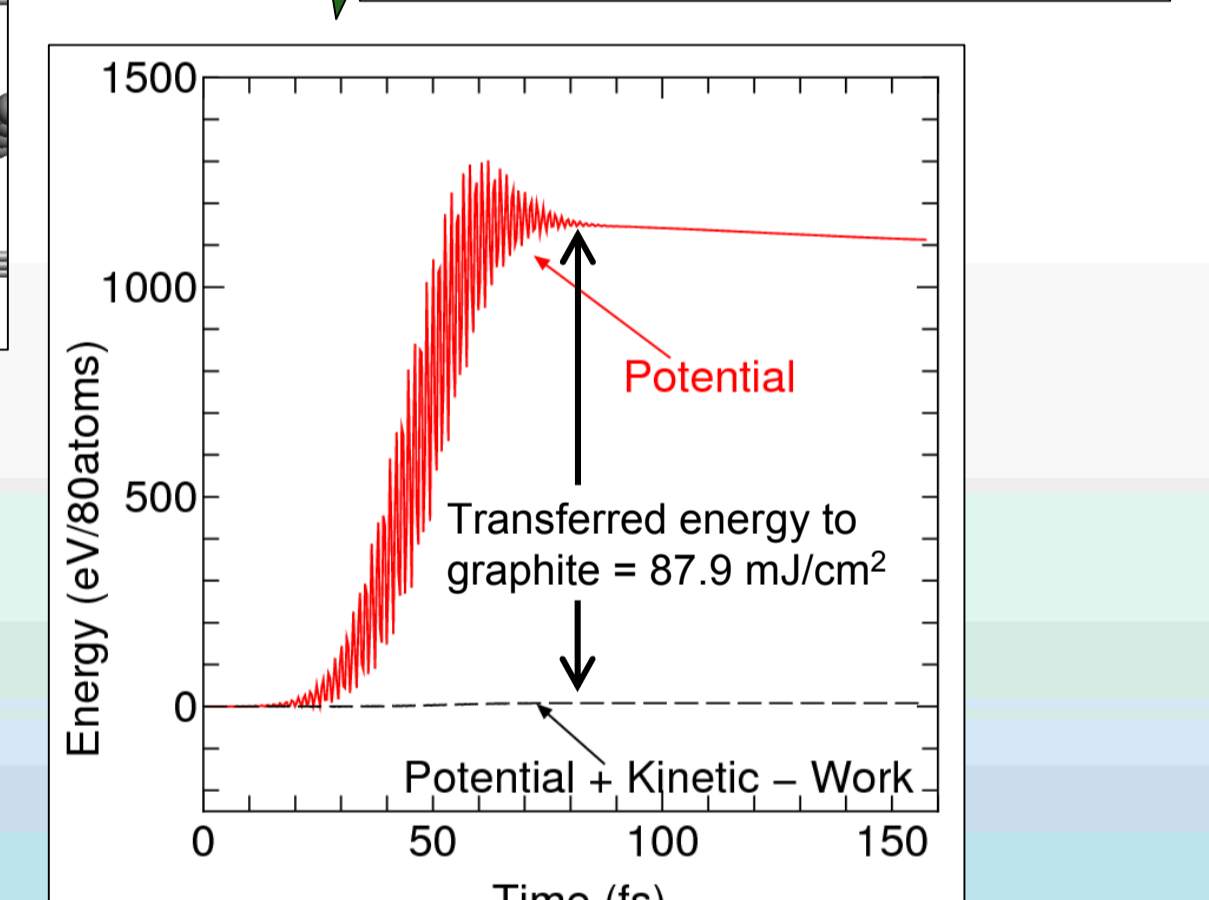
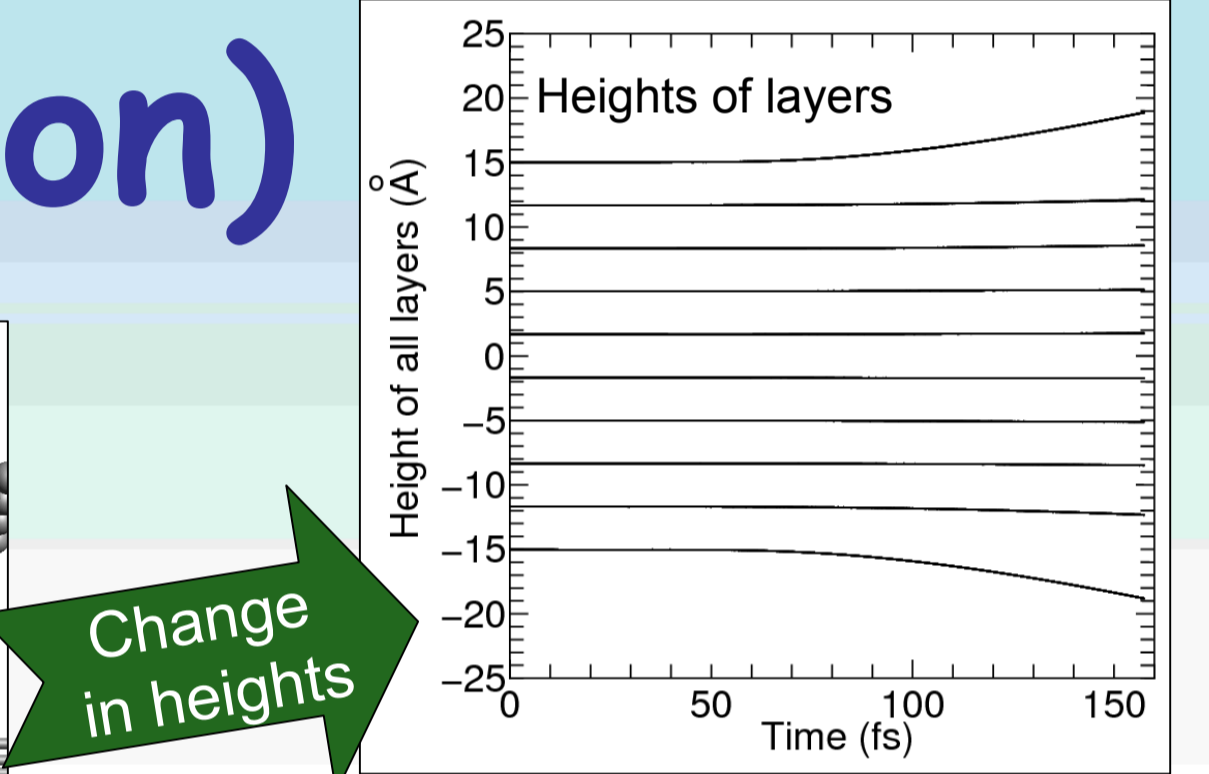
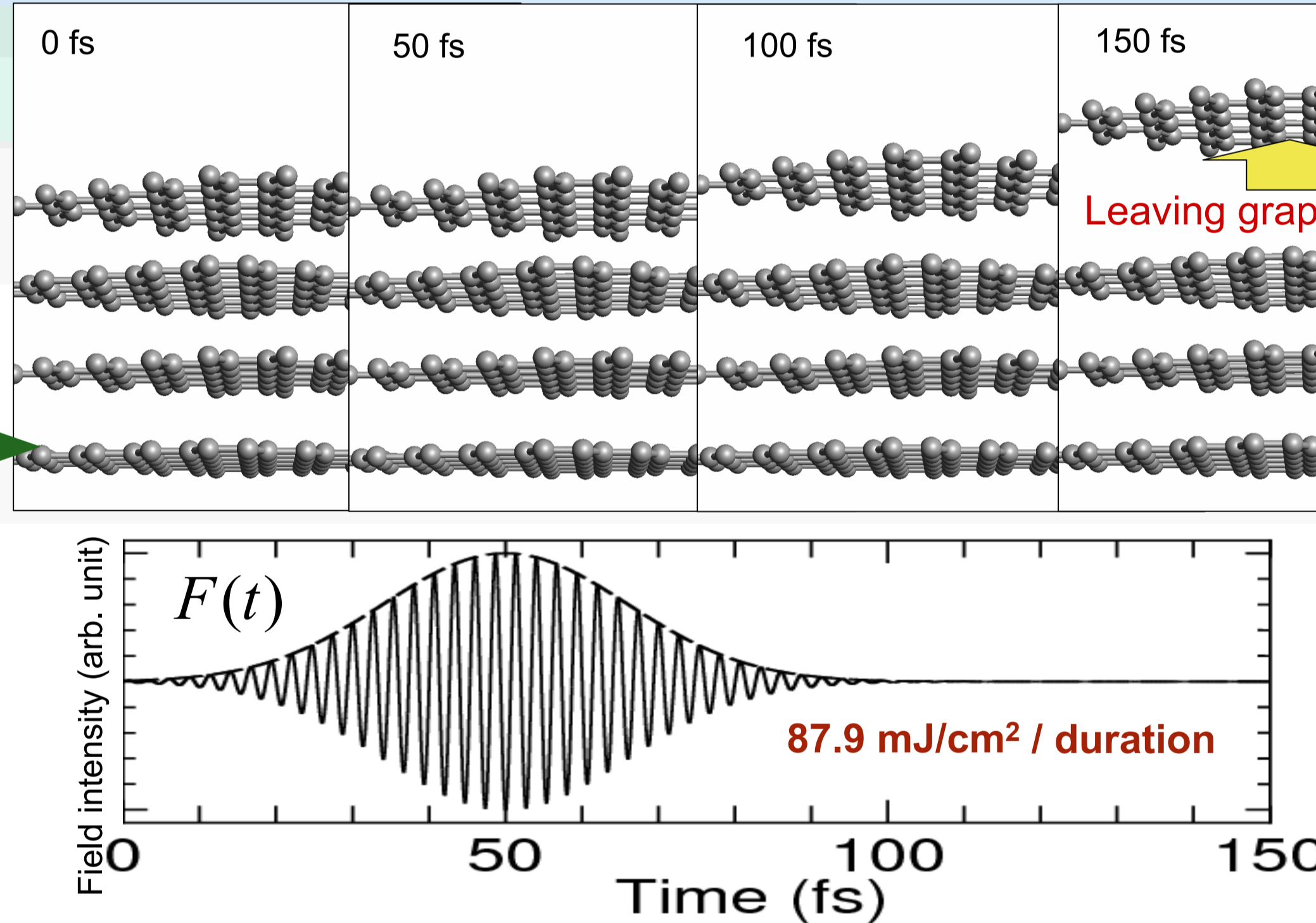


### Computational conditions

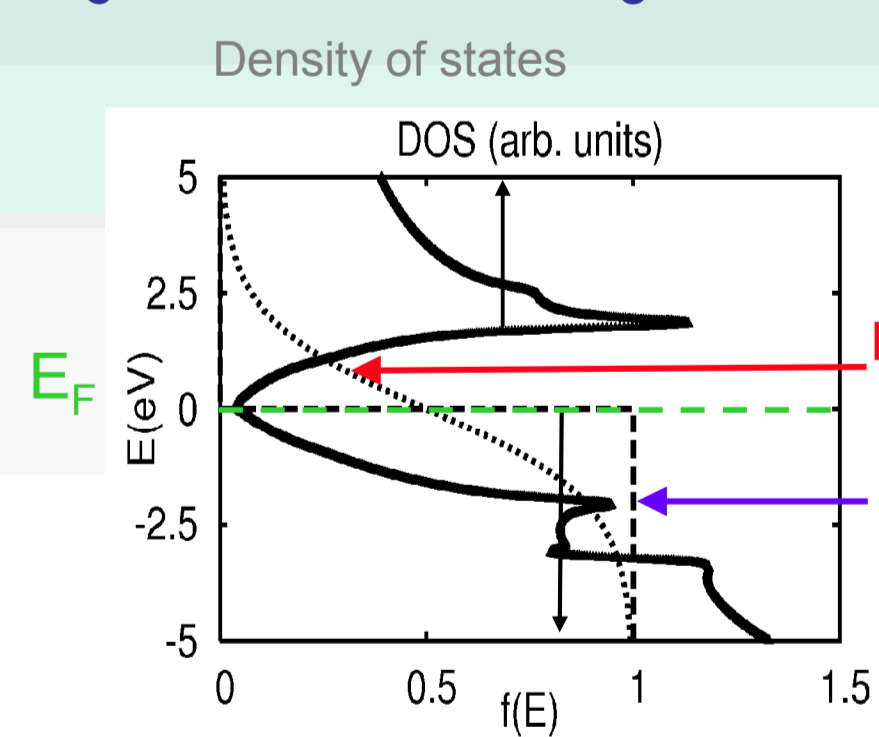
Plane wave basis Ecut=60Ry  
Troullier-Martins PPs  
Single k-point  
Sugino-Miyamoto code - O. Sugino and Y. Miyamoto PRB (1999) (2002)  
Periodic E-field (Sawtooth type)  
Check the conservation rule - Y. Miyamoto and H. Zhang PRB77, 165123 (2008)

Slab geometry of AB-stacked graphene 10-layers and 2x2 lateral cell

$$i\hbar \frac{d\psi_n}{dt} = \left( H_{KS} + V_{ext}(\vec{r}, t) \right) \psi_n$$



## Beyond pico second dynamics (DFT-MD simulation)

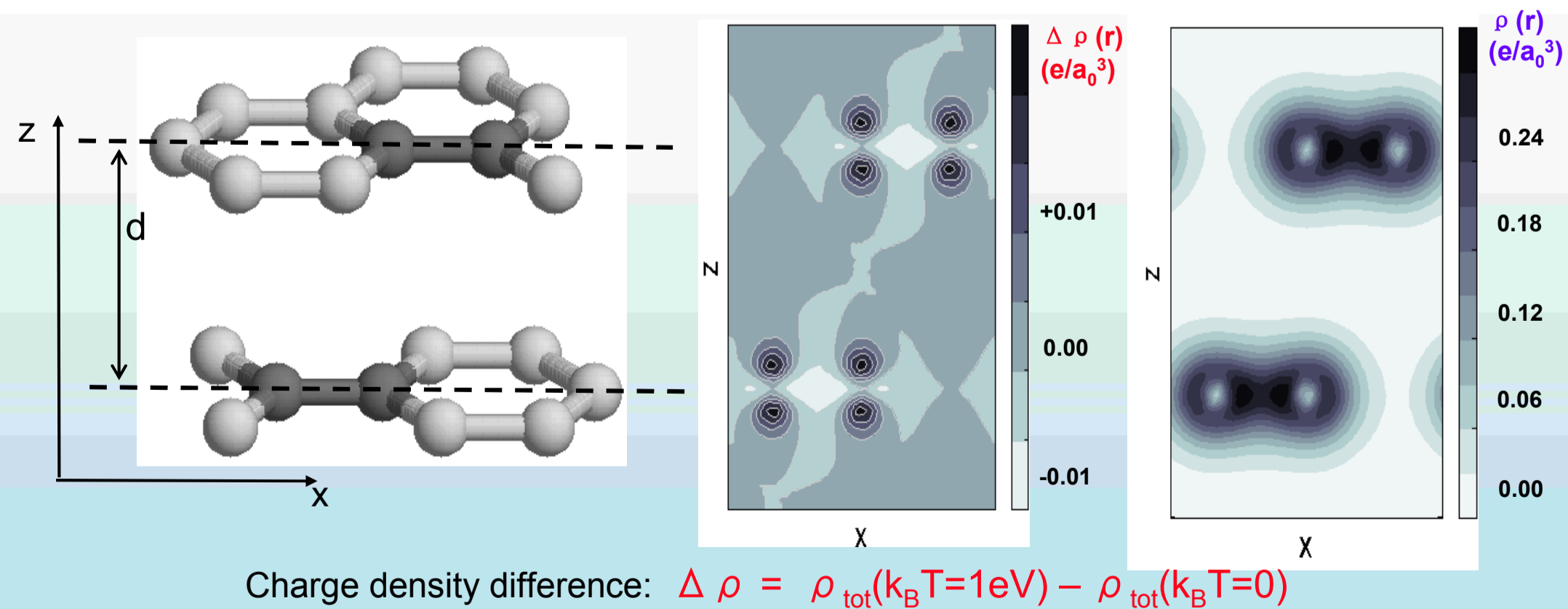


Artificially change occupations assuming electron temperature

➤ Occupy previously empty states in the DOS above  $E_F$

➤ Occupying  $2p_z$  states causes interlayer attraction

➤ Net contraction:  $\Delta d_z \approx -0.04 \text{ \AA}$



Charge density difference:  $\Delta \rho = \rho_{tot}(k_B T=1eV) - \rho_{tot}(k_B T=0)$

## Conclusions

1. Mono-layer graphene peels off by a laser-shot → A new way to graphene formation(!)
2. Longer term dynamics derived from electronic excitation gives lattice contractions
3. Computational prediction for controlled change will be given

## Acknowledgements

All of TDDFT-MD calculations under pulse shot were made by using the Earth Simulator

