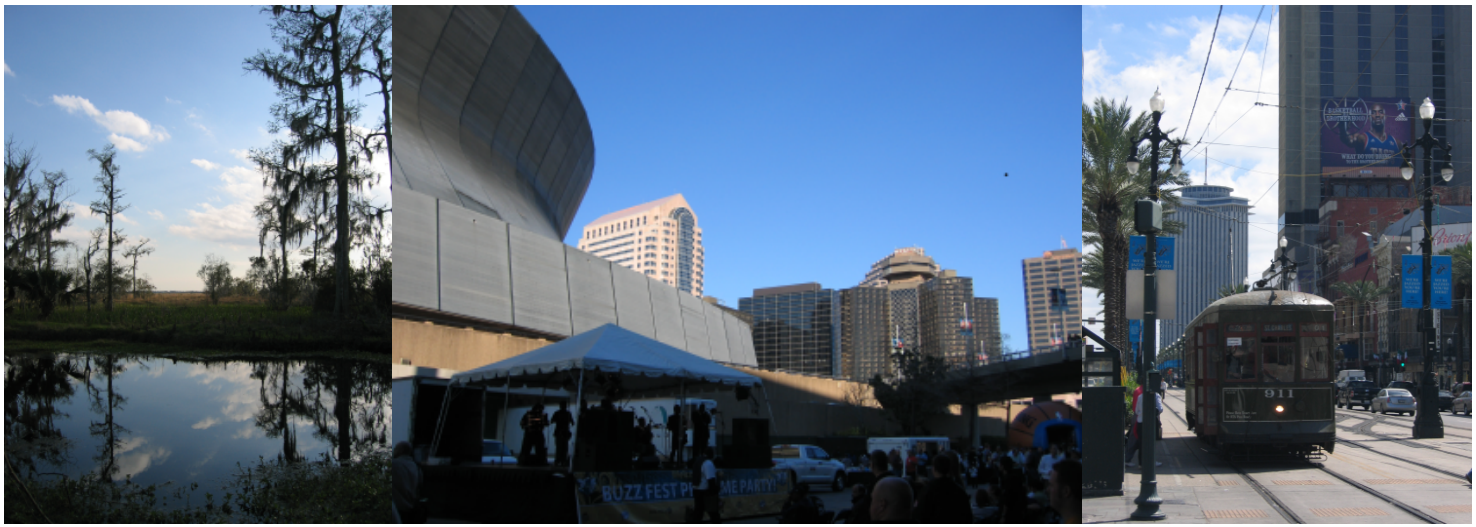
APS March Meeting 2008

R. Hambach

28. 03. 2008

Outline



Graphene-Tutorial

Topic: **Will Carbon Replace Silicon?**
The Future of Graphitic Electronics?
(presentations will become available online)

Graphene-Tutorial I

James Meindl (Georgia Tech)
Beyond the silicon roadmap, what is needed: can carbon-based electronics do the job

- Si chip performance + productivity improved mainly by scaling down
- driving technique: optical nanolithography
- ITRS Roadmap 2007-2022
  main problems (challenges for graphene)
  - maximum battery power
  - size of input/output pads
  - heat transfer
- CNT as wires, but problems with positioning
- graphene ribbons

Graphene-Tutorial II

Millie Dresselhaus:
Graphite, from fullerenes to nanotubes to graphene
nice historical overview (see slides)

- characterization of CNT and graphene by Raman (strong radial breathing mode: 1 CNT $\approx$ Si bulk)
- excitons in small CNTs

Nanoribbons

- again Raman spectroscopy (also RBMs?, chirality?)
- speculation about excitonic effects in small ribbons

Outlook

- CN-tubes is expanding field, towards applications
- GN-ribbon become expanding, learn from tubes!

Graphene-Tutorial III

Phillip Kim (Columbia)

Transport in Graphitic Carbon Nanostructures

ballistic transport

- but practically very impure samples (graphene)
- low temp.: GaAs has much larger mean-free-path
- BUT at room temp.: Graphene is better

type of Defects

no point defects in graphene itself but adsorbates from air, electric traps from substrate, ripples

challenges for CNT-ribbons

- better growing conditions
- controlling edges (they mainly determine transport)

Graphene-Tutorial IV

Walt de Heer (GIT)

Graphene based electronics: epitaxial Graphene

- special technique for growing graphene on SiC (few layer graphite on Si-face)
- the few layers are decoupled from each other (due to small rotation angle)
- substrate induced gap (devices, tuning by gate-volt.)
- toy systems: quantum interference in rings, pseudo-spin experiments, ...
- Carbon oxide (semicond., shottky barrier)

Graphene electronics is NOT only single layer electronics!

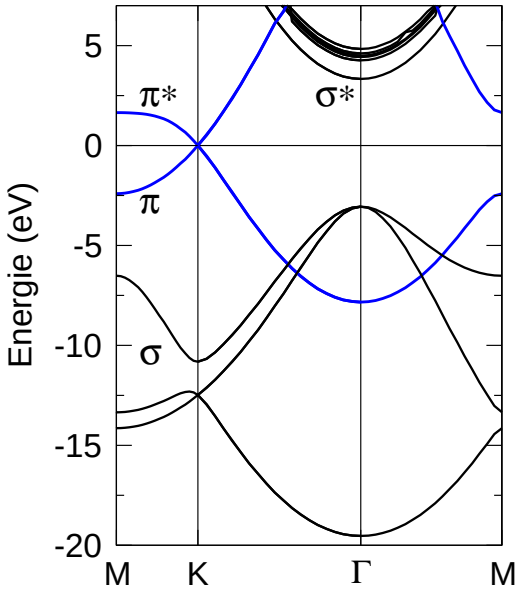
- few layers can be still like isolated graphene
- even 50 layer graphene is NOT equal to graphite

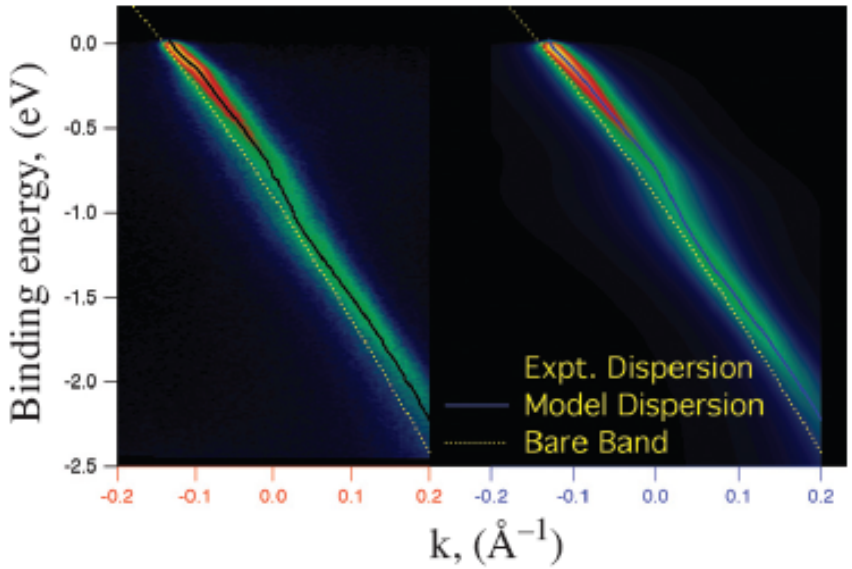
Kink in Band-Structure

Aaron Bostwick *B28.00013 : Symmetry breaking in epitaxial graphene probed by ARPES*

Controversy: kink in linear band dispersion

1. kink-model (MB-effects)
2. gap-model (due to substrate influence)





Kink in Band-Structure

Aaron Bostwick *B28.00013 : Symmetry breaking in epitaxial graphene probed by ARPES*

Evidence for model (1)

- photoemission experiments, shape of Fermi contours [A. Bostwick et al, New J. Phys. **9**, 385 (2007)]
- kink shifts with doping (=¿ model with plasmon)

Reason for observed gap in (2)

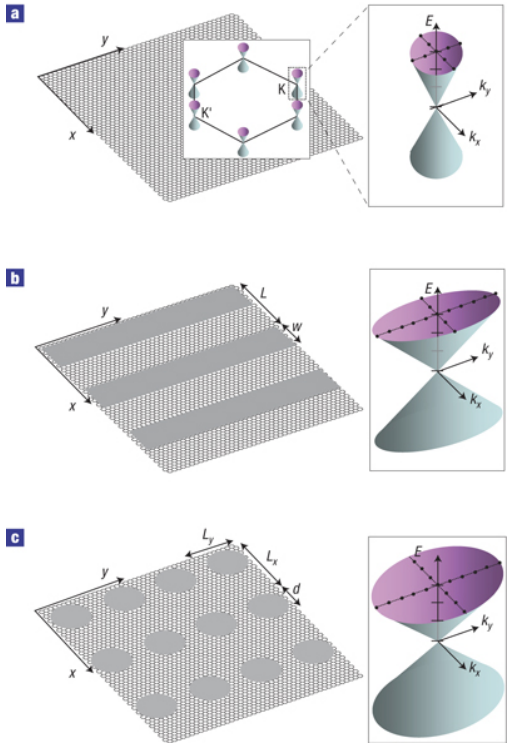
- different samples with small flakes of graphene
- gap openening due to finite size effects ?

see also [Nature **412**, 510 (2001)]

Graphene

Steven Louie: *A28.00002 : Photophysics of Nanostructures: Tubes, Sheets, and Ribbons*

Kronig-Penney superlattice on Graphene



[S. Louie, Nature Physics **4**, 213 (2008)]

Graphene

Steven Louie: *A28.00002 : Photophysics of Nanostructures: Tubes, Sheets, and Ribbons*

Kronig-Penney superlattice on Graphene

- renormalization of band-dispersion by periodic potential
- linear, but direction dependent slope (unchanged in direction of periodicity, up to 0 velocity perpendicular)

[S. Louie, Nature Physics **4**, 213 (2008)]

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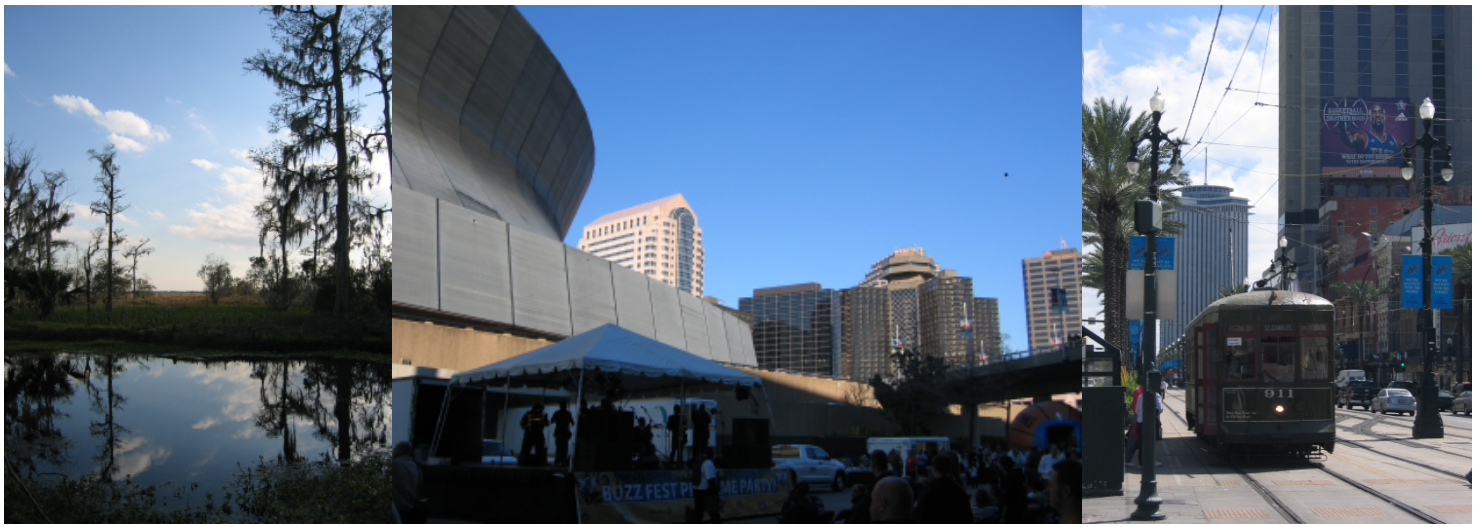

Excitonic effects I

Jack Deslippe, Steven Louie, Tony Heinz:
A28.00003: Effective One-Dimensional Electron-Hole Interaction in Single-Walled Carbon Nanotubes

semiconducting SWCNT [J. Deslippe, Nature]

- very large excit. binding energies, high intensities
- 1D quantum model for e-h interaction (ring charges)
- Antiscreening in SWCNT

metallic SWCNT

- excitons! small binding energies
- from line-shape analysis

BN tubes, Si nanowires, and graphene ribbons

- excitonic effects in ribbons, charge transfer exciton

Excitonic effects II

J. Kas, M. Prange, F.D. Vila, Y. Takimoto, J.J. Rehr:
X37.00002 : First principles calculations of optical and x-ray spectra from atomic coordinates alone

Inelastic losses in x-ray absorption with self energy correction + vibrational properties

- ϵ^{-1} calculated at $q = 0$ and extrapolated to finite momenum transfer (multipole model) [Phys. Rev. B **76**, 195116 (2007)]
- vibrational properties from DFT (Debye-Waller-Factors)

$\Rightarrow$ slightly better in XANES

$\Rightarrow$ improved EXAF quantitatively

"Combined BSE and TDDFT approach for x-ray absorption calculations" [Phys. Rev. B **71**, 165110 (2005)]

double wall CNT

Morinobu Endo: *B30.00001 : Novel Functions in Double Walled Carbon Nanotubes*

Double wall CNT remain interesting

- much lower degradation
- chemical modification of outer tube
- intercalation (storage, linear atom chains)
- doping into special sites may be interesting for applications

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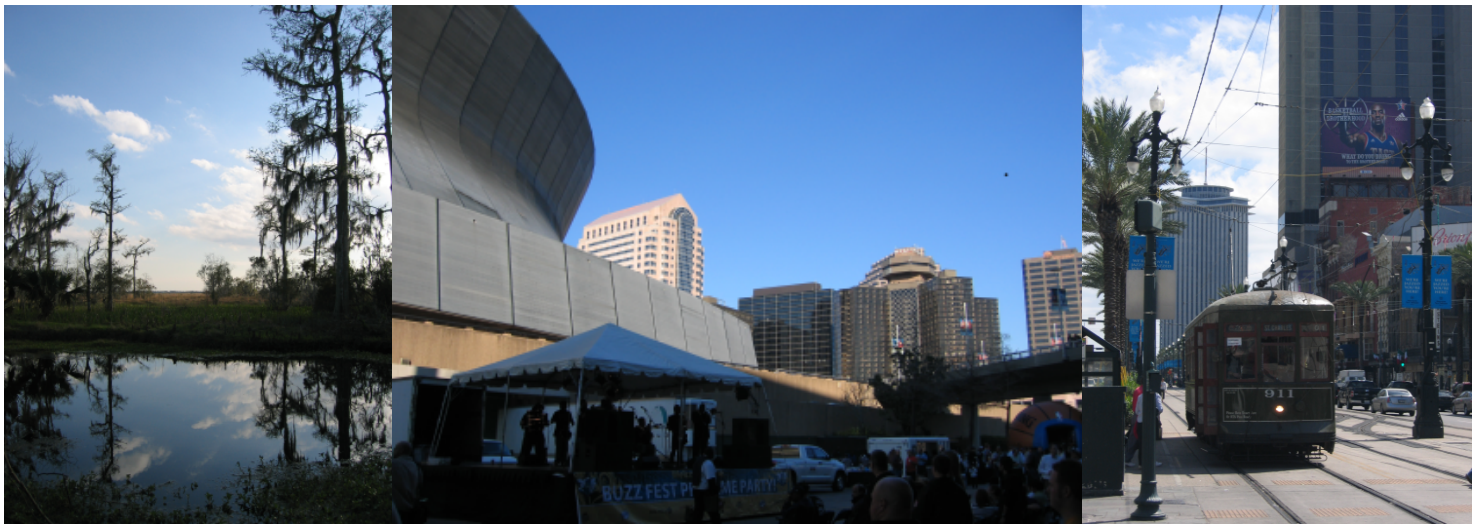

DFT

Walter Kohn: *D1.00001: Nearsightedness in Density Functional Theory* [PNAS, vol. **102**, 11635 (2005)]

John P. Perdew:
D1.00005: Restoring the Density-Gradient Expansion for Exchange in a GGA for Solid and Surfaces PBEsol improves equilibrium properties of densely-packed solids and their surfaces
[J.P. Perdew, A. Ruzsinszky, G.I. Csonka, O.A. Vydrov, G.E. Scuseria, L.A. Constantin, X. Zhou, K. Burke]

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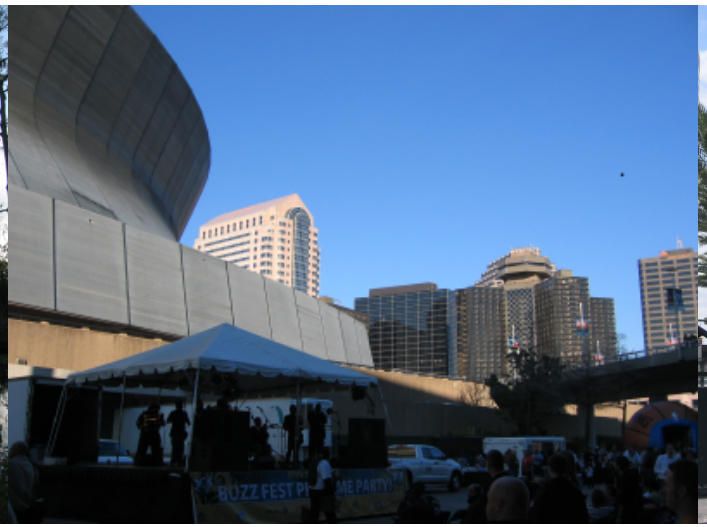

Strongly Correlated Sys. I

Sergey Savrasov: *A3.00002 : Computational Approaches for Strongly Correlated Materials: an Electronic Structure Theory Perspective.*
new techniques, a spectral density functional theory, which considers total free energy as a functional of a local electronic Green function

Strongly Correlated Sys. II

Hamann, Vanderbilt: *D13.00001: Maximally-localized Wannier functions for GW quasiparticles*
combined the WANNIER90 code for MLWF with the self-consistent GW capabilities of the ABINIT code until now for Si and perovskite $SrZrS_3$

Strongly Correlated Sys. III

Rei Sakuma, Miyake,Aryasetiawan: *D13.00003: All-electron GW calculation of vanadium dioxide*
GW calculation of metallic and insulating vanadium dioxide using a full-potential LMTO basis set. The calculations show that it is crucial to take into account both the frequency dependence and the off-diagonal elements of the self-energy...

Other

Ann E. Mattsson:
S13.00003: Accurate and fast DFT calculations with the AM05 functional

- AM05 functional is on a regular semi-local GGA form
- performs exceptionally well for solids and surfaces. [R. Armiento and A. E. Mattsson, Phys. Rev. B **72**, 085108 (2005).]

- H35.00003 : Novel acoustic surface plasmons on Cu(111) (Karsten Pohl) [Nature 448, 57 (2007)]
- H35.00004 : Thickness dependent plasmon excitation and damping in metallic thin films (Zhe Yuan) [Phys. Rev. B 73, 155411 (2006)]
- H24.00007 : Anisotropic plasmon excitation and dispersion of Ag nanowires on Cu(110) (I. Senevirathne)

- H35.00007 : Controlling surface plasmons and local field by two-dimensional arrays of metallic nano-bottles (Hei lu)
- X28.00004 : Study of the absorption spectra of periodic hole arrays (Dimitrios Koukis) surface plasmon-wave manipulation (diffraction, focussing, switching) [Appl. Phys. Lett. 91, 083115 (2007)]
- U29.00007 : Electronic screening in graphite (James Reed) [Phys. Rev. Lett. 92, 237401 (2004)]