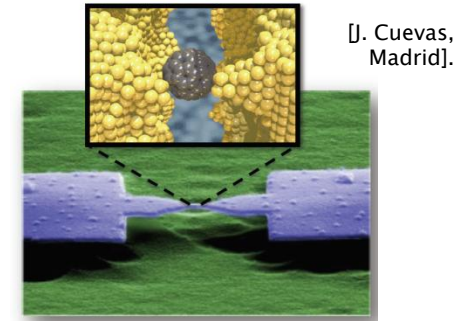
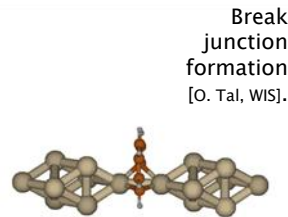


Parallelized electronic transport calculations in real space

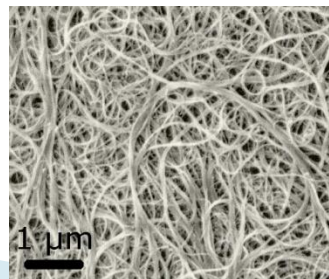
Baruch Feldman, Leeor Kronik, Weizmann Institute of Science
Oded Hod, Tel Aviv University
Tamar Seideman, Northwestern University

American Physical Society March Meeting
Room 326, Session M24: Electronic Structure Methods I
Baltimore, March 20, 2013

Motivation + Background

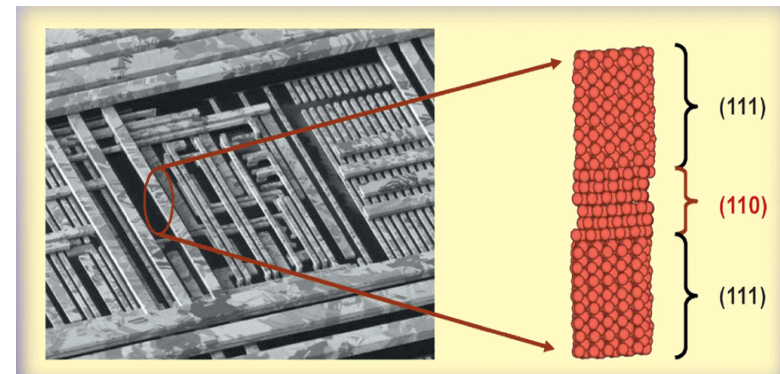


- ▶ Molecular electronics
 - Bulk electrodes coupled to atomic/molecular-scale system
 - Important from basic & applied science perspectives
 - Transport calculations
 - Landauer theory, NEGF
- ▶ Need for **larger** calculations
 - Organic / crystal interfaces
 - Include electrode, gate atoms
 - CNT ropes/bundles, graphene
 - Multiple geometries



CNT
bundle
[Wikipedia].

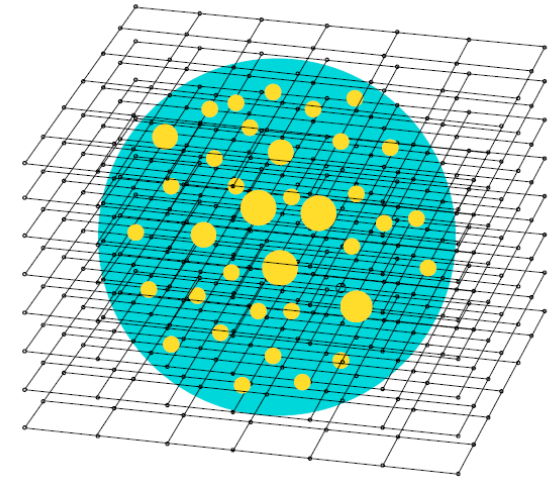
- ▶ Highly parallel method
 - Real space DFT + NEGF
 - Also: better convergence, boundary conditions
 - Previous real space NEGF
 - Ono, Tsukamoto, *et al*, *J. Phys.: Cond. Mat.*, 2011
 - Kong, Tiago, Chelikowsky, *PRB*, 2006



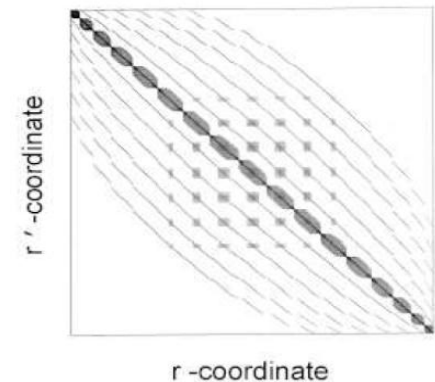
CPU Interconnect simulation – nm scale crystallites,
grain boundaries [B. Feldman et al., *Phys. Stat. Solidi B*,
2010].

Advantages of Real Space (e⁻ structure & transport)

- ▶ *Iterative* eigensolution (for both e⁻ structure and transport)
 - Bottleneck: Mat-Vec operation
 - $H |\psi\rangle$
 - Communication only needed for off-diagonal blocks *between cores*
- ▶ Amdahl's Law:
Total time = Overhead + Communication + Parallelizable CPU work
- ▶ Problem very sparse in real space (both e⁻ structure and transport)
 - H_{KS} Diagonals:
 - V_{KS}
 - Part of ∇^2
 - Off-diagonals:
 - (Finite diff expansion) part of ∇^2
 - Pseudopotential (*cutoff* radius R_c , above right)
 - Sparseness depicted at right



Real space grid in PARSEC, with domain boundary and atoms
[Chelikowsky, *J Phys D*, 2000; Kronik, Makmal, *et al.*, *Phys Stat Solidi B*, 2006].

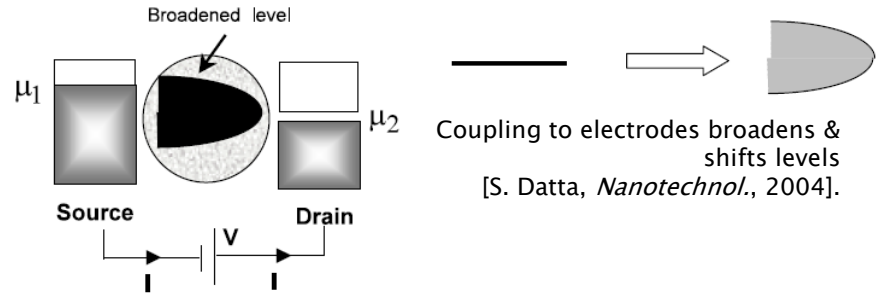


Sparseness of typical H_{KS}
[courtesy Y. Saad].

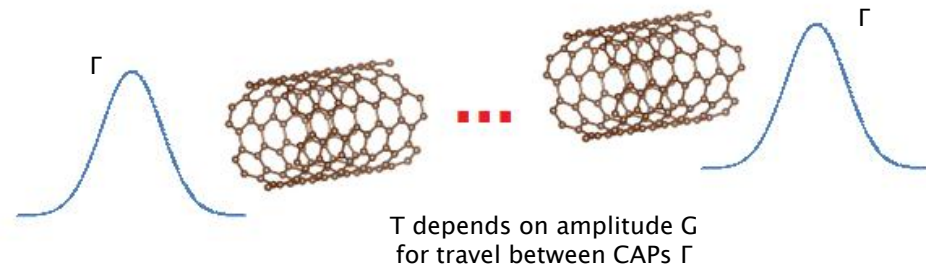
Real-Space Transport + CAPs

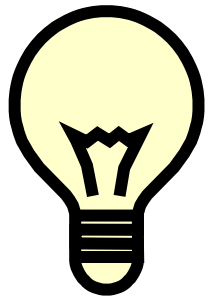
- ▶ Transport in real-space with PARSEC
- ▶ Current depends on transmission $T(E)$ across nanoscale system
 - T depends on Green function $G(E) = (E - H)^{-1}$
 - S. Datta, *Electronic Transport in Mesoscopic Systems*, 1995

- ▶ Coupling to electrodes **broadens**
+ **shifts** energy levels
 - $E \rightarrow \text{Complex}$
 - Broaden levels
 - Finite lifetime



- ▶ Represent infinite electrodes by complex absorbing potentials (CAPs; below right)
 - $V_{KS} \rightarrow V_{KS} + i\Gamma$
 - Absorbs incoming ψ
 - Here: Γ Gaussian - tune parameters to electrode
 - **NOW** must find $G(E) = [E - (H_{KS} + i\Gamma)]^{-1}$
- ▶ Real space: **Large** inversion problem!
- ▶ Advantage: Highly parallelizable
 - Suitable for large systems!





Inversion by Diagonalization Approach

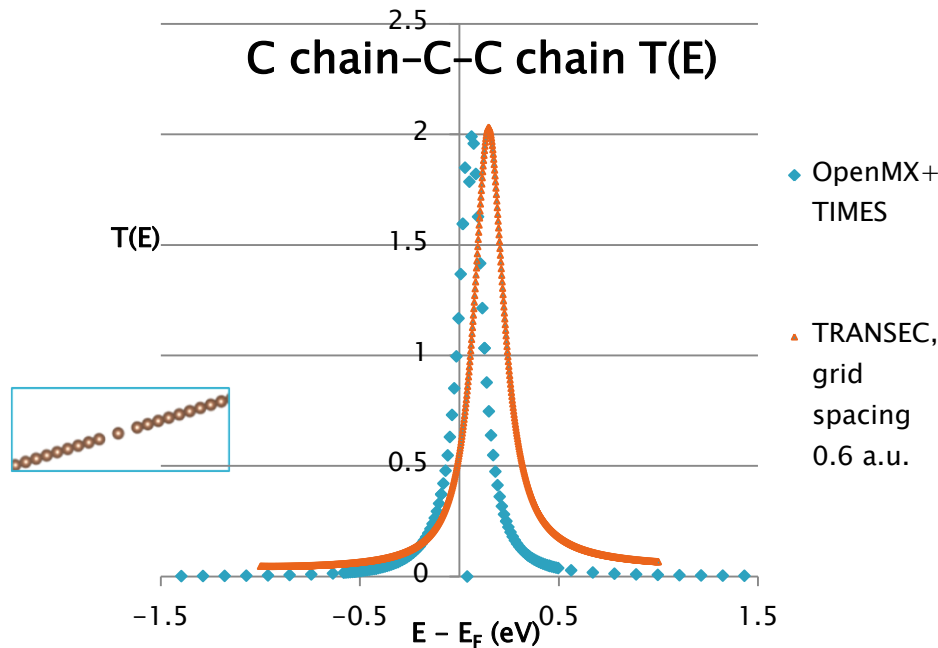
- ▶ Transport controlled by bias window around Fermi level:

$$\text{Bias window} = E_F \pm V/2$$

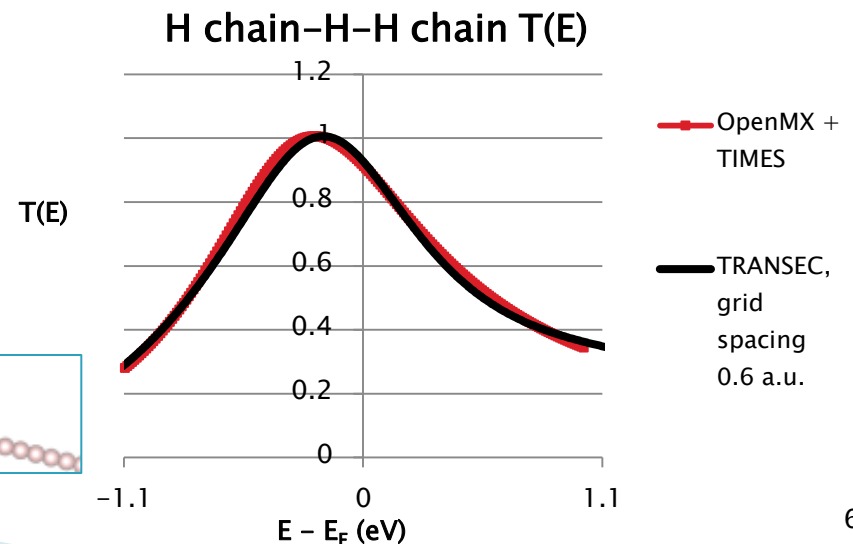
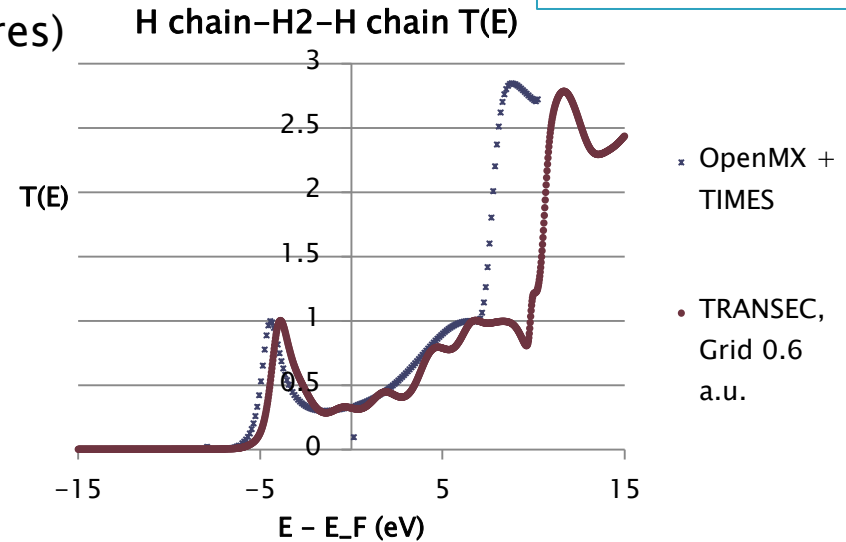
- \Rightarrow Redundant to find entire inverse
- ▶ Diagonalize $(H_{KS} + i \Gamma) \longrightarrow \epsilon$
 - Iterative eigensolver
- ▶ Inversion of $[E - (H_{KS} + i \Gamma)]$ becomes trivial
 - $1/(E - \epsilon)$
 - Only need ϵ “near” bias window
 - All energies E in one shot!

Benchmarks: Atomic chain tests

- ▶ Good agreement with other codes
 - ~ 0.1 eV (like comparing band structures)

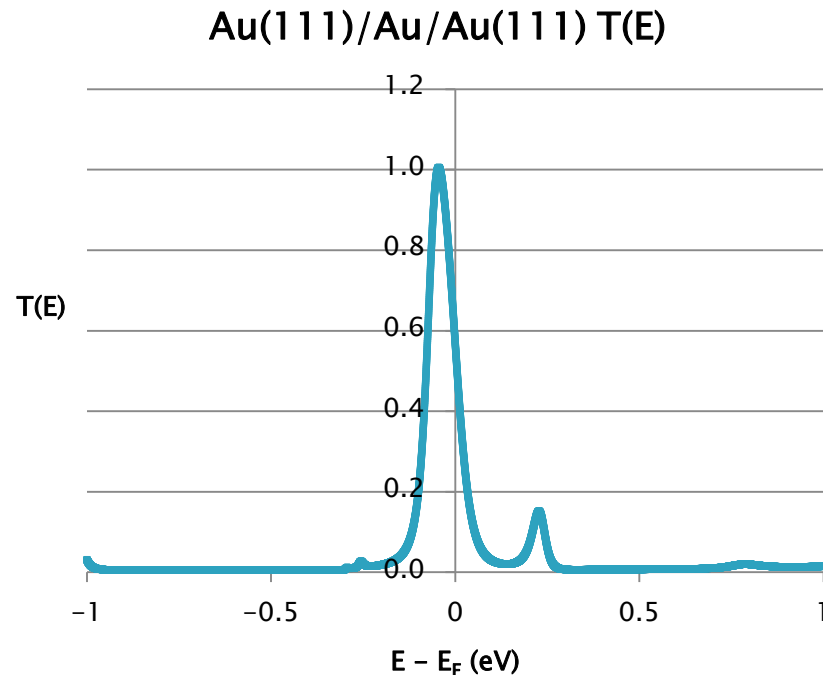
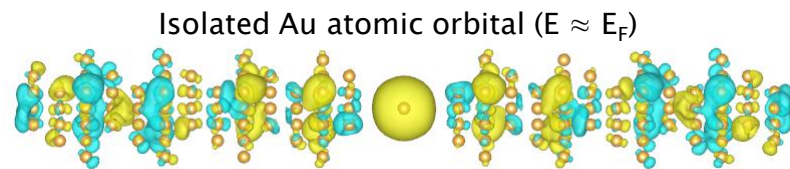
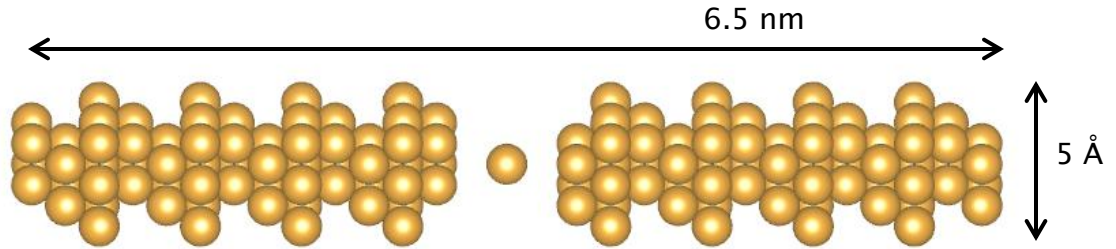


- ▶ Matches analytical expectations
 - Peak height = # modes
 - Width depends on gap



Results: Au (111) / Au / Au(111) system

- ▶ Very large Au leads
 - ~145 Au atoms
 - Allow decay of both CAPs
- ▶ $T(E)$ peak of height 1 at $E = E_F$
 - Conductance channel through isolated Au atom (right center)



Summary

- ▶ Need *larger* nanoscale conduction calculations (NEGF)
- ▶ Real-space method + CAP's
 - Energy diagonalization
 - Highly parallelizable
- ▶ Atomic chain tests
 - Good agreement
- ▶ Au electrodes
 - Results for Au(1 1 1)
 - Au + BDT molecule underway

Thank you!

Leeor Kronik, Oded Hod, Tamar Seideman, Ariel
Biller, Mark Vilensky, NWU IT, Kronik group