Outline:

- **A short review of state-of-the-art;**
- **DFT atomistic methods;**
- **The NEGF-DFT implementation;**
- **Applications of NEGF-DFT;**
- → **Quantum mechanic forces during current flow;**
- **Summary: outlook to the near future.**

The total energy functional in DFT:

$$\begin{aligned} E_{\rm tot} &= T_{\rm KS} + \tfrac{1}{2}\int d\mathbf{r}d\mathbf{r}'\frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} + +E_{\rm XC}[\rho(\mathbf{r})] \\ &\int d\mathbf{r}\,\rho(\mathbf{r})V_{\rm ion-el}(\mathbf{r}) + \textstyle\int d\mathbf{r}\,\rho(\mathbf{r})V_{ext} + E_{\rm ion-ion}[\{\mathbf{R}_I\}], \end{aligned}$$

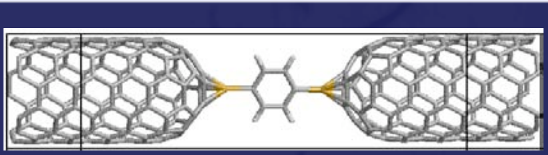
$$E_{\rm tot} = E_{\rm BS} + \delta E_{\rm H} + \delta U_{\rm XC} + E_{\rm ion-ion}[\{\mathbf{R}_I\}],$$

$$\begin{aligned} E_{\rm BS} &= \sum_{i=1}^{N} E^i \\ \delta E_{\rm H} &= -\frac{1}{2}\int d\mathbf{r}\,\frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \\ \delta U_{\rm XC} &= \int d\mathbf{r}\,\rho(\mathbf{r})\left(\frac{E_{\rm XC}(\rho(\mathbf{r}))}{\rho(\mathbf{r})} - V_{\rm XC}(\rho(\mathbf{r}))\right) \\ E_{\rm ion-ion} &= \sum_{I\neq J}\frac{Z_I Z_J}{|\mathbf{R}_I-\mathbf{R}_J|}. \end{aligned}$$

$$E^i = \int d\mathbf{r}(\psi^i(\mathbf{r}))^*\left\{\frac{-\nabla^2}{2} + \int d\mathbf{r}\frac{\rho(\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|} + V_{\rm XC}(\rho(\mathbf{r}))V_{\rm ion-el}(\mathbf{r}) + V_{\rm ext}(\mathbf{r})\right\}\psi^i(\mathbf{r}).$$

The KS eigen-values

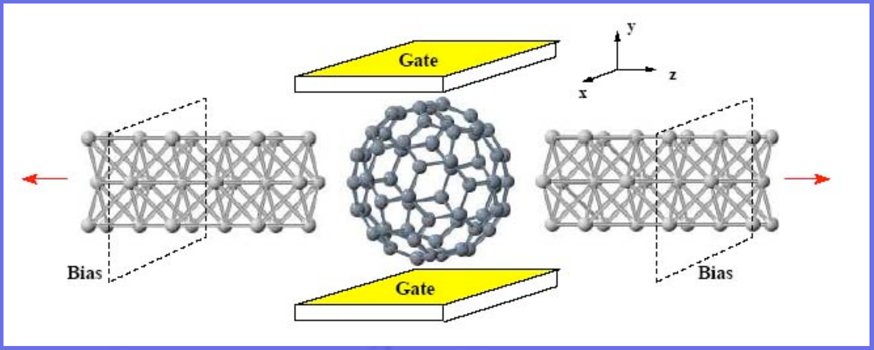
Forces for open system during current flow



- When the external bias is not too large, the system is near an equilibrium ground state, the total energy of the scattering region is well defined.
- By computing the steady-state energy density matrix, one can calculate quantum mechanical forces within the NEGF-DFT framework.
- Such an approximation can be established in more firm theoretical footing **(T. N. Todorov, Philos. Mag. B 80, 421 (2000); PRL 92, 176803(2004)).**

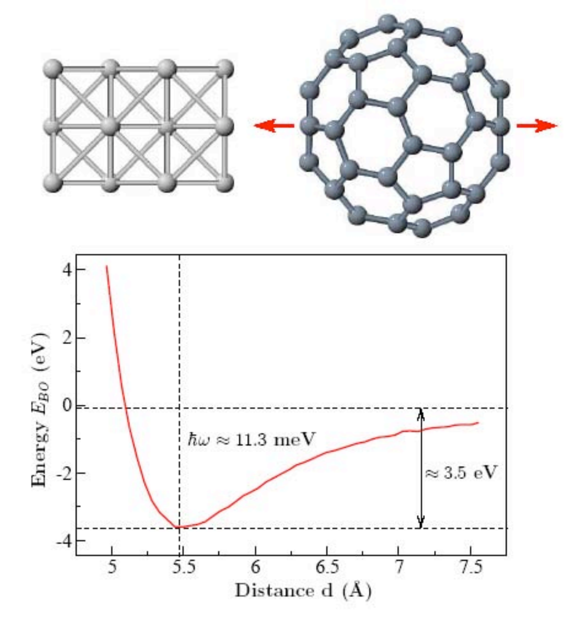
- But we have to re-formulate all things in terms of NEGF so that the non-equilibrium statistics is properly accounted for. This turns out to be a very tedious problem to do **(Sergeuuv, Roubtsov, H.G. PRL 95, 146803(2005)).**

First, a simple and direct calculation



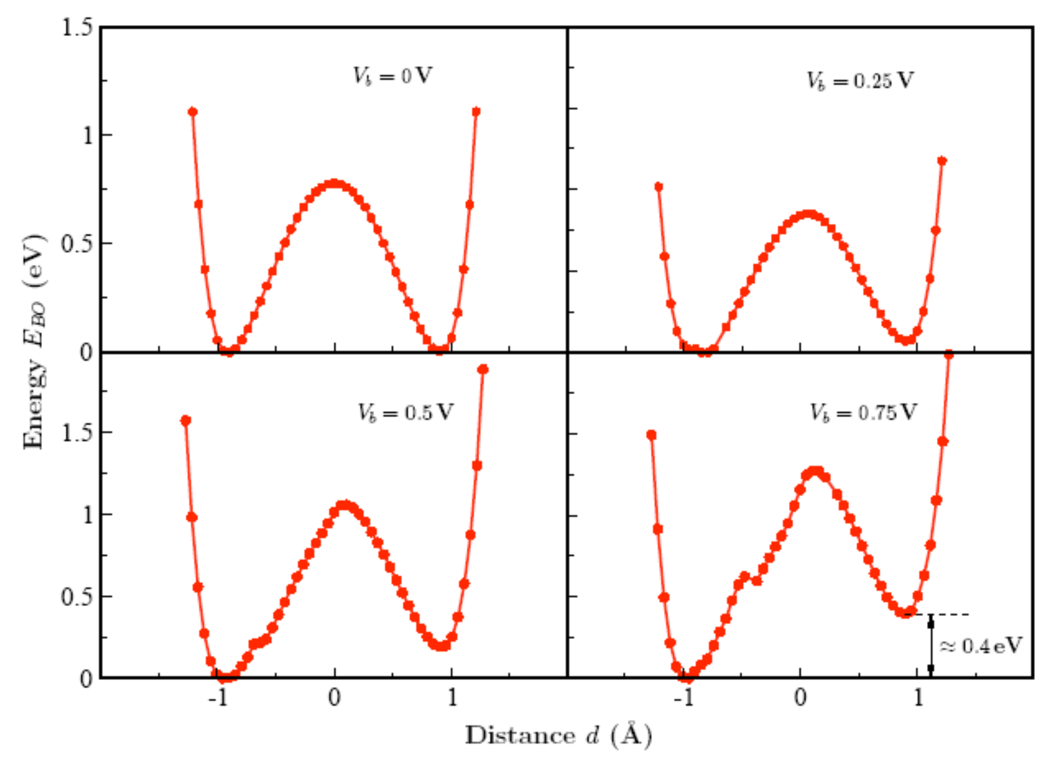
A C60 and a wire will make a equilibrium bond.

This can be computed by total energy.



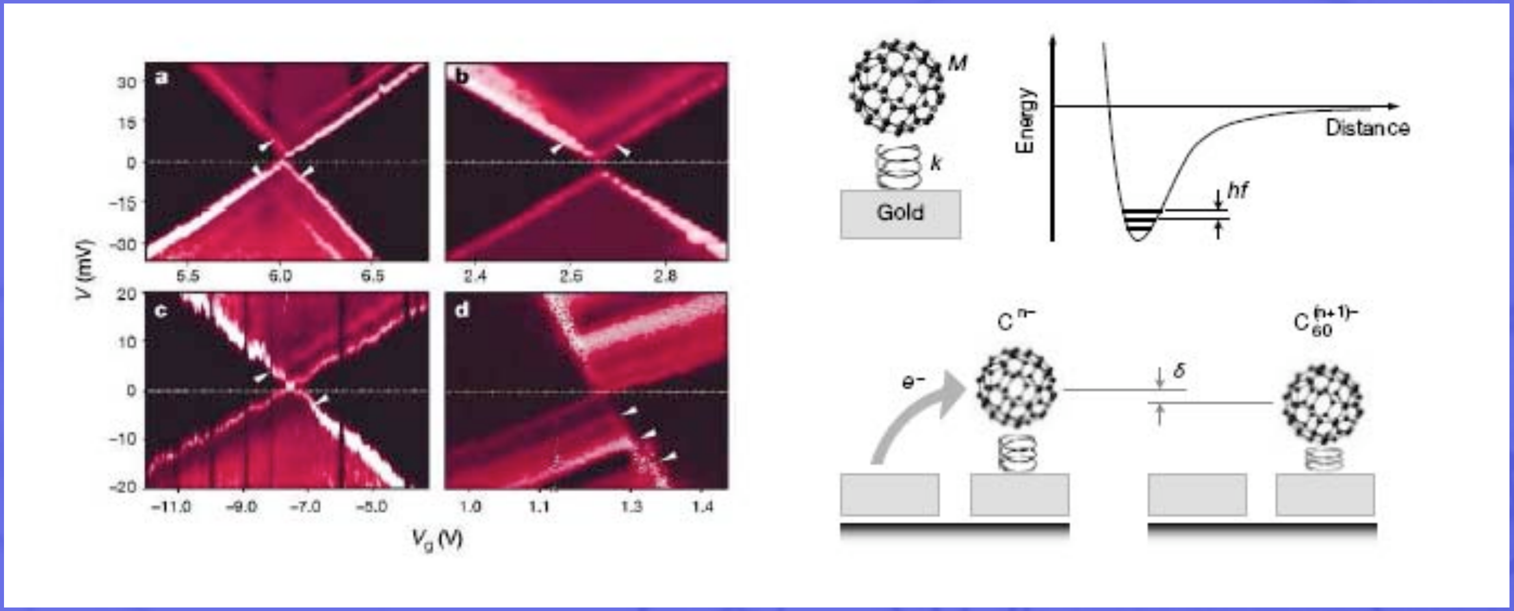
C60 sits in between two leads

When the lead-lead distance is large enough, a bias voltage pushes the C60 to one energy minimum.



The vibrational quantum for the center-of-mass motion inside one minimum is found to be 8.5meV, and this does not change much for different bias.

Experiment of Park etal:



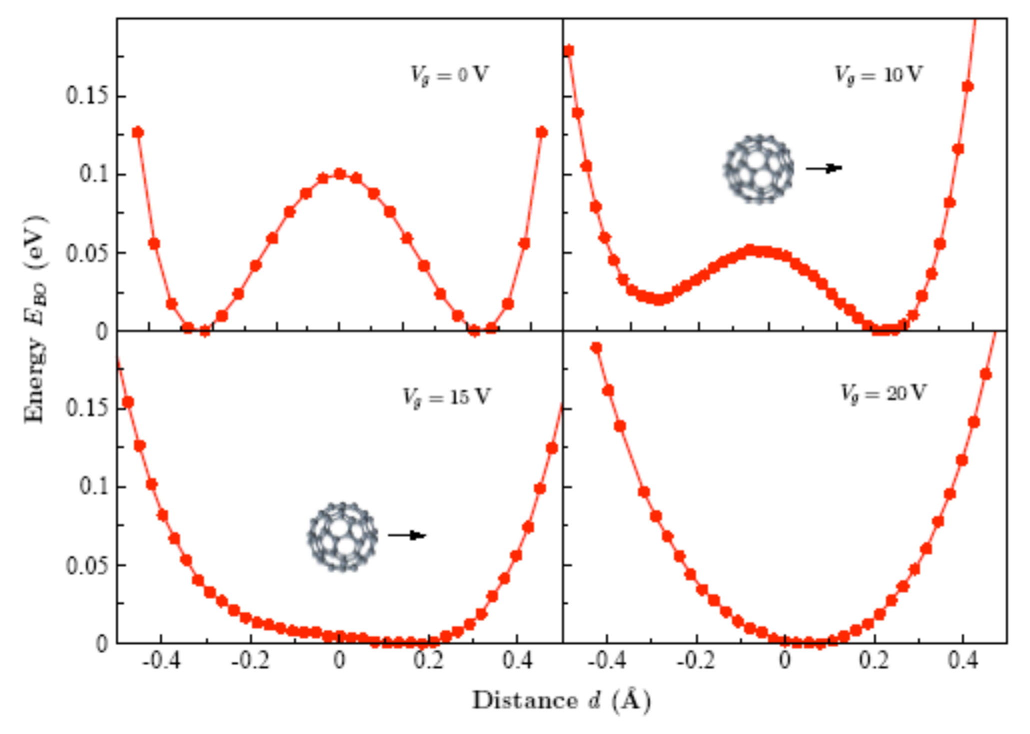
Transport measurement suggested a vibrational quantum for center-of-mass motion to be ~5meV.

H. Park etal, Nature, 407, 57 (2000)

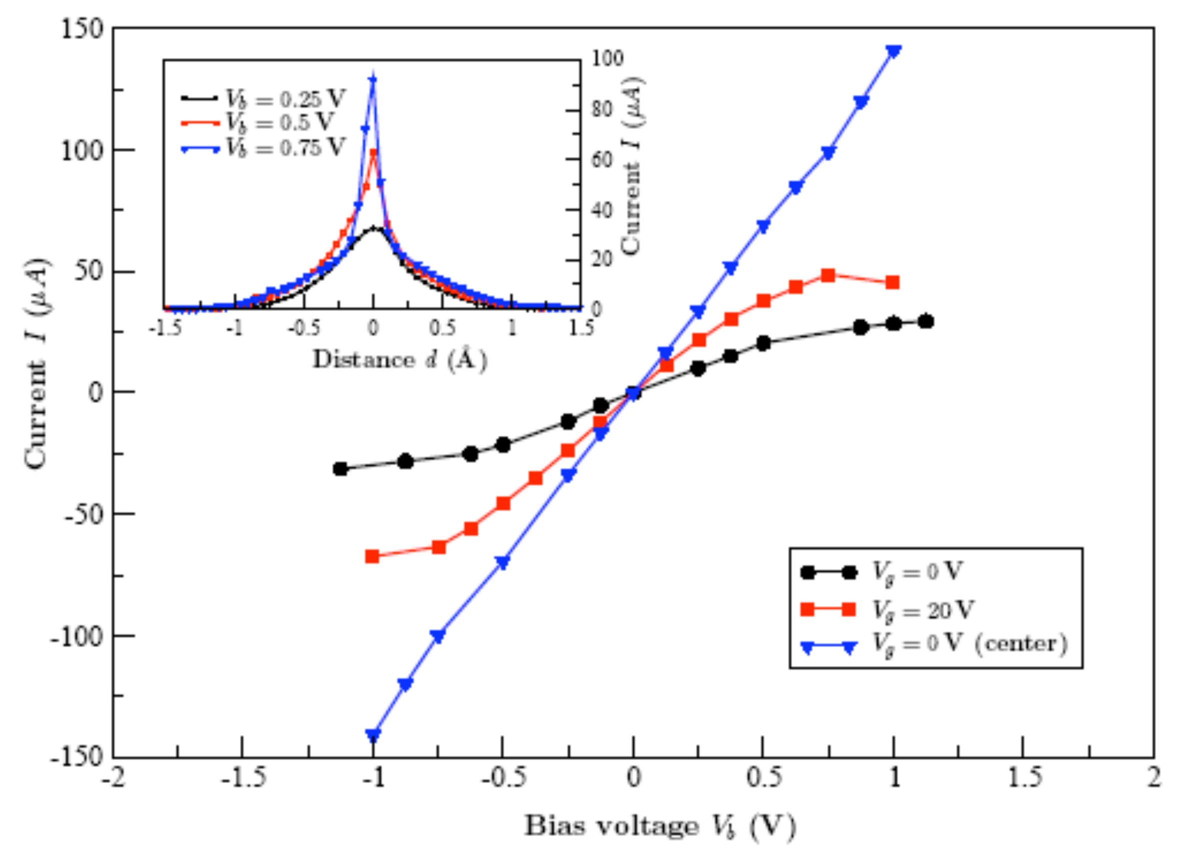
Effect of a gate voltage

A positive gate voltage attracts charge from the leads toward C60.

It levels the middle barrier, gives rise to large effect in transport.



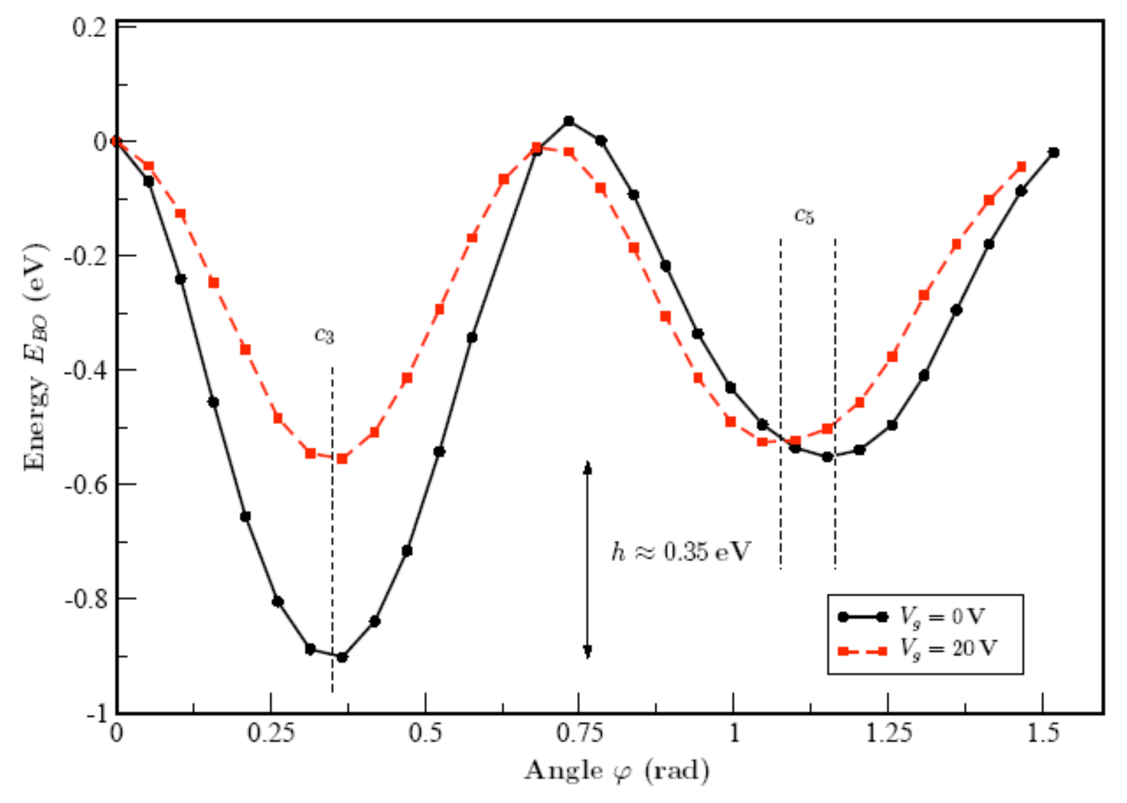
Transport effect due to the center-of-mass motion:



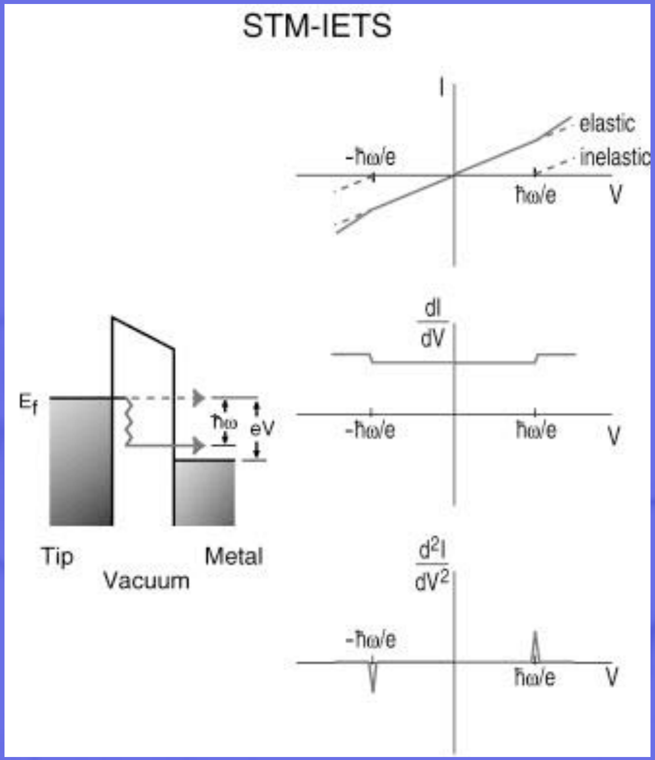
Rotational motion:

Energy is lower when hexagons face the lead (c3).

A gate voltage, somehow, levels the two minima.



Second, a general full NEGF-DFT analysis



Inelastic Electron Tunneling Spectroscopy (IETS) detects this.

Current driven by voltage.

↓

Excitation of vibrational mode

↓

Opening of inelastic electron tunneling channel

↓

Change in the conductance *(dI/dV)*

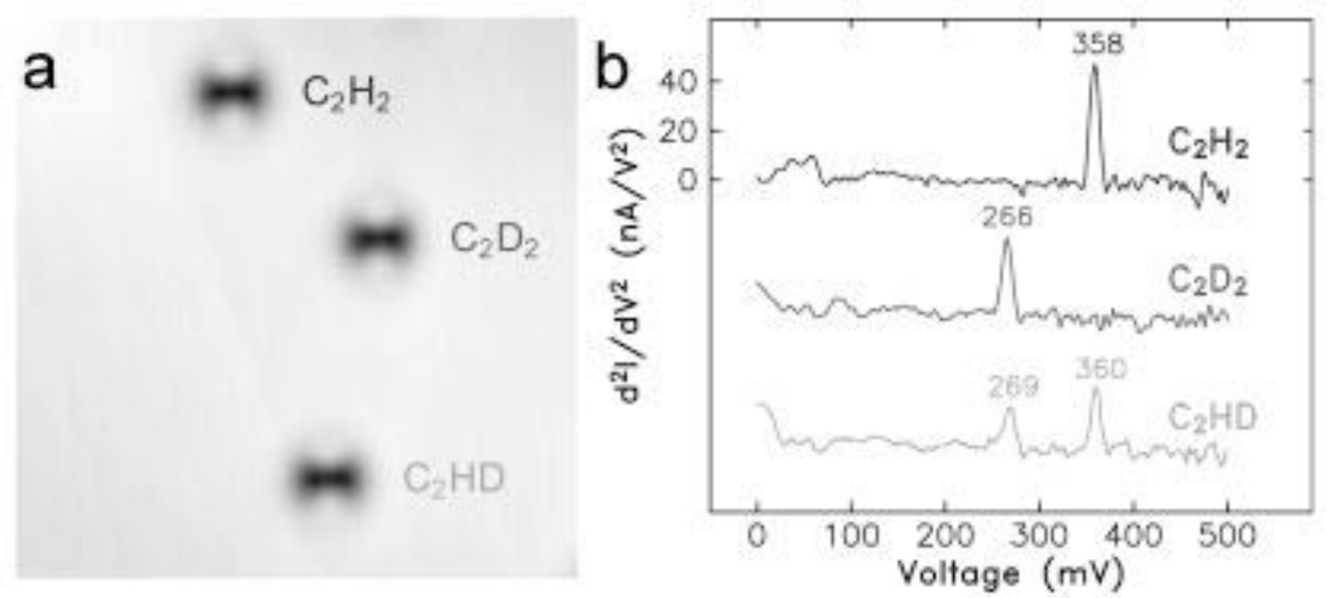
W. Ho *et al.*, J. Chem. Phys., 117,11033, (2002)

Inelastic tunnelling spectroscopy with STM

W. Ho (2002)

Acetylene $(\mathrm{H-C\equiv C-H}\ \text{ or }\ \mathrm{D-C\equiv C-D}\ \text{ or }\ \mathrm{D-C\equiv C-H})$

on Cu (001) at 8 K



only C-H or C-D stretching mode is resolved

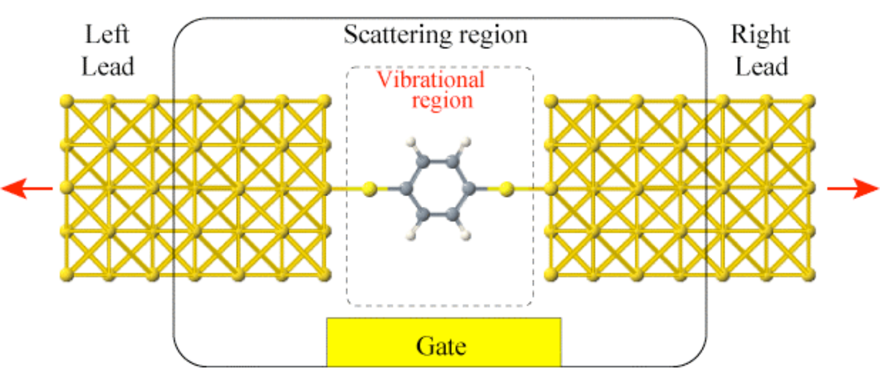
Relevant questions:

How to predict "active" vibrational modes of the molecule that contribute to inelastic conductance ?

What are the selection rules for e-p coupling ?

Which modes couple to which scattering states at what bias voltage ?

Definition of problem: vibrations of molecule in the junction



Typical system: a molecule in contact with two electrodes

Total Calculation Box: N atoms

↓

Scattering region: N_c atoms

↓

Vibrational region : N_k atoms

Scattering region includes some portion of the leads: extended molecule

← We consider atoms inside this box

Determine vibration spectra: from NEGF-DFT

Step 1: solve Kohn-Sham equation for electronic Hamiltonian of device by NEGF-DFT:

$$\hat{H}_{\mathrm{K-S}}[\rho] = \hat{T} + \hat{V}_{\mathrm{ps}} + \hat{V}_{\mathrm{H}} + \hat{V}_{\mathrm{xc}}$$

Step 2: compute Born-Oppenheimer total energy of the scattering region:

$$E_{\mathrm{B-O}} = \mathrm{Tr}\,(\hat{\rho}\,\hat{H}_{\mathrm{K-S}}) - \frac{1}{2}\int d\mathbf{r}\, V_{\mathrm{H}}(\mathbf{r})\,\rho(\mathbf{r}) - \int d\mathbf{r}\, V_{\mathrm{xc}}(\mathbf{r})\,\rho(\mathbf{r}) + E_{\mathrm{xc}}[\rho] + \frac{e^2}{2}\sum_{j,j'=1}^{N}\frac{Z_j\,Z_{j'}}{|\mathbf{R}_j - \mathbf{R}_{j'}|}$$

Step 3: Compute dynamical matrix which give vibrational eigenvectors and eigenfrequencies (normal modes):

$$\sum_{j,\beta}\frac{1}{\sqrt{M_i\,M_j}}\,\frac{\partial^2 E_{\mathrm{B-O}}[\mathbf{R}_1,\,\cdots,\,\mathbf{R}_N]}{\partial R_{i,\alpha}\,\partial R_{j,\beta}}\Big|_{\mathbf{R}_{i'}=\mathbf{R}_{i'}^{(0)}}\,\mathrm{e}_\beta(\nu,\,j) = \omega_\nu^2\,\mathrm{e}_\alpha(\nu,\,i)$$

The electron-phonon coupling strength:

$$\hat{H}_{\rm tot} \;=\; \hat{H}_{\rm K-S}\,[\,\mathbf{R}_j^{(0)}\,] \;+\; \hat{H}_{\rm vib}\,[\,\hbar\omega_\nu;\,\mathbf{R}_j^{(0)}\,] \;+\; \hat{H}_{\rm e-mv}\,[\,g_\nu,\,\mathbf{e}_\nu,\,\hbar\omega_\nu;\,\mathbf{R}_j^{(0)}\,]$$

Kohn-Sham Hamiltonian (electrons) :

$$\hat{H}_{\rm K-S}\,[\,\rho\,] \;=\; \hat{T} \;+\; \hat{V}_{\rm ps} \;+\; \hat{V}_{\rm H} \;+\; \hat{V}_{\rm xc}$$

Quantized molecular vibrations---“phonons” (ions) :

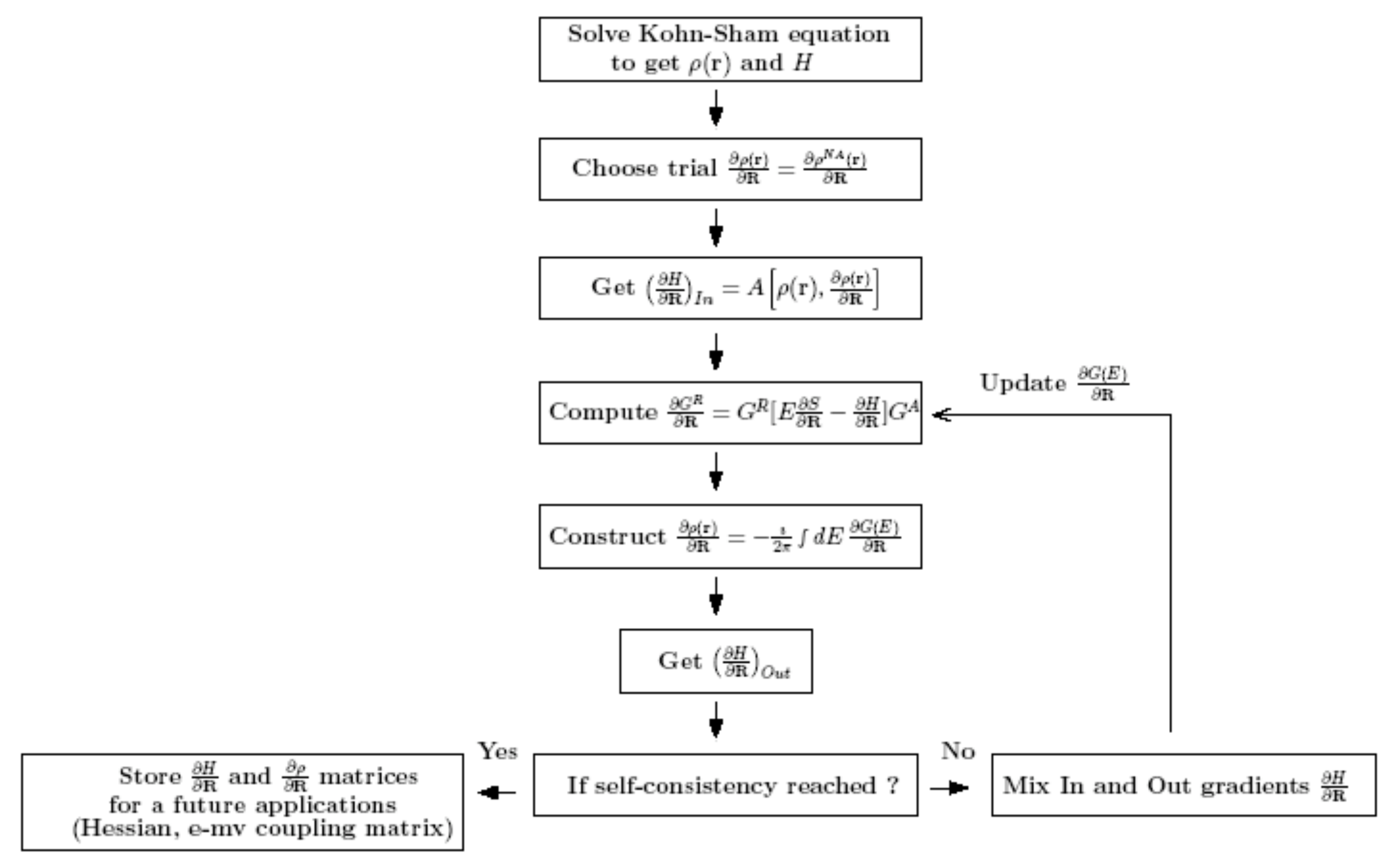
$$\hat{H}_{\rm vib} \;=\; \sum_\nu \hbar\omega_\nu/2 \;+\; \sum_\nu \hbar\omega_\nu\,\hat{b}_\nu^\dagger\,\hat{b}_\nu, \qquad \nu \;=\; 1,\,2,\,\cdots,\,3N_k$$

Interaction Hamiltonian :

$$\hat{H}_{\rm e-mv} \;=\; \sum_\nu \hat{g}_\nu\,(\,\hat{b}_\nu^\dagger \;+\; \hat{b}_\nu\,), \qquad \hat{g}_\nu = \sum_{j\,\subset\,\text{vibr. box}} \sqrt{\frac{\hbar}{2M_j\,\omega_\nu}}\;\mathbf{e}(\nu,\,j)\,\frac{\partial}{\partial\,\mathbf{R}_j}\,\hat{H}_{\rm K-S}\,[\,\rho(\mathbf{r})\,]\Big|_{\mathbf{R}_i=\mathbf{R}_i^{(0)}}$$

e-p coupling strength

Some implementation details:



Solve Kohn-Sham equation to get $\rho(\mathbf{r})$ and H

Choose trial $\frac{\partial\rho(\mathbf{r})}{\partial\mathbf{R}} = \frac{\partial\rho^{NA}(\mathbf{r})}{\partial\mathbf{R}}$

Get $\left(\frac{\partial H}{\partial\mathbf{R}}\right)_{In} = A\left[\rho(\mathbf{r}), \frac{\partial\rho(\mathbf{r})}{\partial\mathbf{R}}\right]$

Compute $\frac{\partial G^R}{\partial\mathbf{R}} = G^R[E\frac{\partial S}{\partial\mathbf{R}} - \frac{\partial H}{\partial\mathbf{R}}]G^A$

Update $\frac{\partial G(E)}{\partial\mathbf{R}}$

Construct $\frac{\partial\rho(\mathbf{r})}{\partial\mathbf{R}} = -\frac{1}{2\pi}\int dE\,\frac{\partial G(E)}{\partial\mathbf{R}}$

Get $\left(\frac{\partial H}{\partial\mathbf{R}}\right)_{Out}$

If self-consistency reached ?

Yes

Store $\frac{\partial H}{\partial\mathbf{R}}$ and $\frac{\partial\rho}{\partial\mathbf{R}}$ matrices
for a future applications
(Hessian, e-mv coupling matrix)

No

Mix In and Out gradients $\frac{\partial H}{\partial\mathbf{R}}$

N. Sergueev, Ph.D thesis, McGill, (2005).

Test on a free BDT molecule: single zeta basis

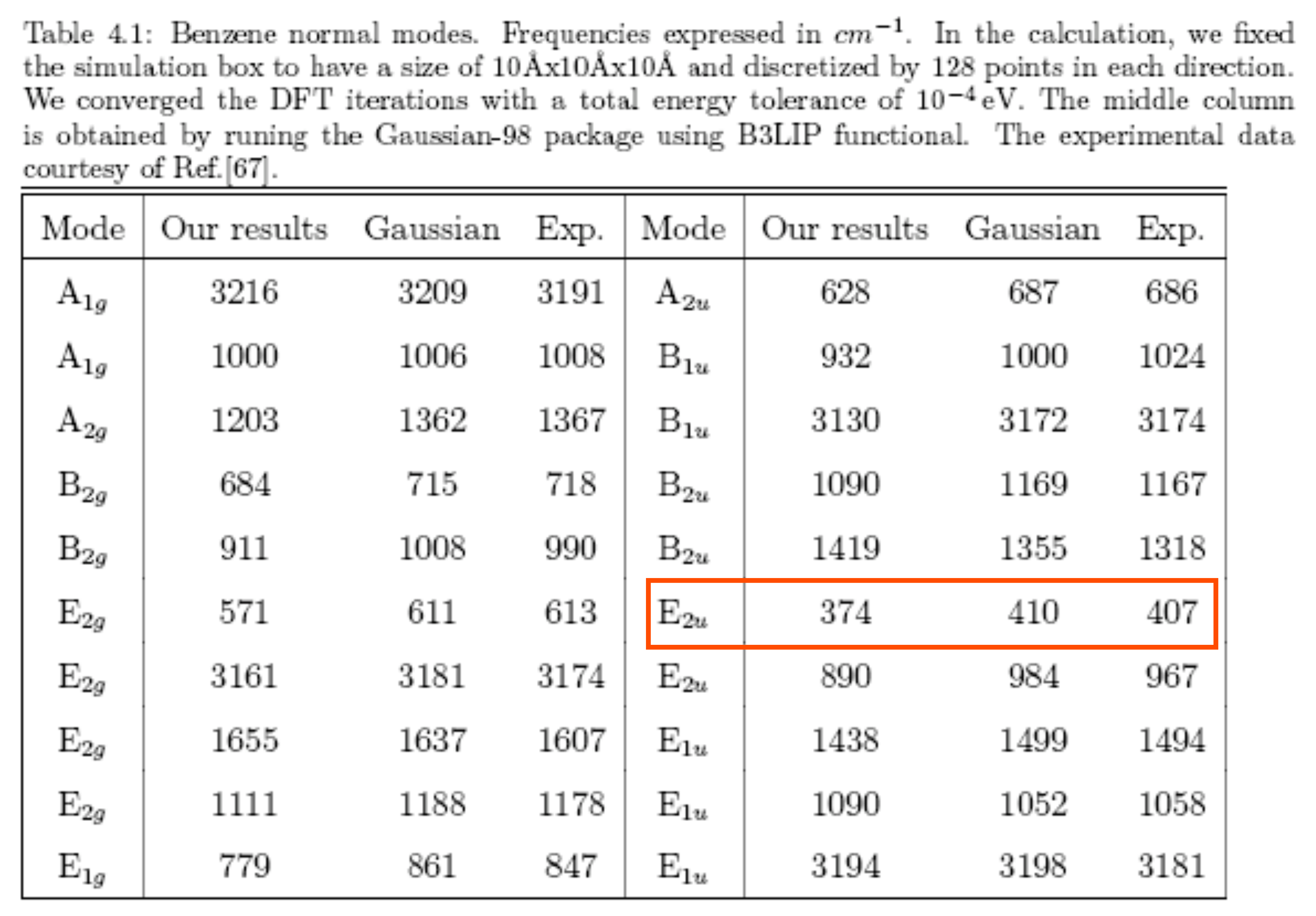


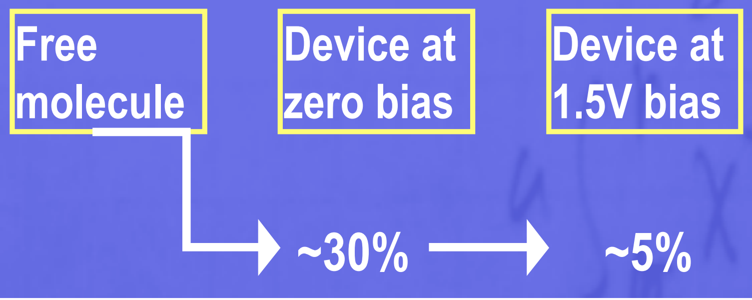
Table 4.1: Benzene normal modes. Frequencies expressed in cm^{-1}. In the calculation, we fixed the simulation box to have a size of 10Åx10Åx10Å and discretized by 128 points in each direction. We converged the DFT iterations with a total energy tolerance of 10^{-4}eV. The middle column is obtained by runing the Gaussian-98 package using B3LIP functional. The experimental data courtesy of Ref.[67].

Mode	Our results	Gaussian	Exp.	Mode	Our results	Gaussian	Exp.
A_{1g}	3216	3209	3191	A_{2u}	628	687	686
A_{1g}	1000	1006	1008	B_{1u}	932	1000	1024
A_{2g}	1203	1362	1367	B_{1u}	3130	3172	3174
B_{2g}	684	715	718	B_{2u}	1090	1169	1167
B_{2g}	911	1008	990	B_{2u}	1419	1355	1318
E_{2g}	571	611	613	E_{2u}	374	410	407
E_{2g}	3161	3181	3174	E_{2u}	890	984	967
E_{2g}	1655	1637	1607	E_{1u}	1438	1499	1494
E_{2g}	1111	1188	1178	E_{1u}	1090	1052	1058
E_{1g}	779	861	847	E_{1u}	3194	3198	3181

8%
error

Vibration spectra of a model device with 1,4 benzenedithiolate molecule

Extra low lying modes show up for 2-probe devices: due to existence of leads which breaks symmetry.



Free molecule

Device at zero bias

Device at 1.5V bias

~30%

~5%

For transport, only a few MO’s are important:

$$\langle \hat{g}_n \rangle (E, E') = \langle \Psi_{sc}(E) | \hat{g}_n | \Psi_{sc}(E') \rangle$$

$$\langle RMO_\alpha | \hat{g}^n | RMO_\beta \rangle$$

Only a few molecular orbitals (MO’s) are important for transmission, all near the Fermi level (some HOMO and LUMO). Therefore, the e-p coupling in transport are most contributed by them.

For transport, off diagonal elements $\alpha \neq \beta$ are almost as important as the diagonal elements.

Dimensionless e-p coupling strength at zero bias

1. Some modes are more important than others.
2. Low lying modes are important.
3. No clear selection rules.

Dimensionless e-p coupling: finite bias

$$\lambda_{\nu}^{(\mathrm{el})}(V_b) = \int_{\mu_R}^{\mu_L} \frac{dE}{V_b}\,\mathrm{DOS}(E)\,\frac{\langle \hat{g}_{\nu} \rangle^2(E,\,E)}{\hbar\omega_{\nu}}$$

$$\lambda_{\nu}^{(\mathrm{inel},\pm)}(V_b) = \int_{\mu_R}^{\mu_L} \frac{dE}{V_b}\,\mathrm{DOS}(E)\,\frac{\langle \hat{g}_{\nu} \rangle^2(E,\,E \pm \hbar\omega_{\nu})}{\hbar\omega_{\nu}}$$

Bias voltage
V_b=1.0V

1. Drastic change in coupling strength.
2. Center of mass modes seem to be important.
3. Value increase by a factor ~5.

E-p coupling strength vs bias voltage:

New scattering states entering bias window, causing e-p coupling to increase.

Important implications to other phenomena.

Sergueev, Roubtsov, H.G PRL 95, 146803(2005)

Computing inelastic current: NEGF-DFT-SCBA:

Step 1: Compute Green's function:

$$G^{\mathrm{R}}(E) = (\, ES - H_{\mathrm{K-S}} - \Sigma^{\mathrm{R}}_{l}(E) - \Sigma^{\mathrm{R}}_{r}(E) \; - \; \Sigma^{\mathrm{R}}_{\mathrm{e-mv}}(E)\,)^{-1}$$

If a systems is at non-equilibrium:

$$G^{<}(E) = i\, G^{\mathrm{R}}(E)\, \Gamma_{l}(E)\, n_{\mathrm{F},\,L}(E)\, G^{\mathrm{A}}(E) + i\, G^{\mathrm{R}}(E)\, \Gamma_{r}(E)\, n_{\mathrm{F},\,R}(E)\, G^{\mathrm{A}}(E) + G^{\mathrm{R}}(E)\, \Sigma^{<}_{\mathrm{e-mv}}(E)\, G^{\mathrm{A}}(E)$$

Step 2: Obtain density matrix

$$\int dE\, G^{<}(E)/(2\pi i) = \hat{\rho} \;\rightarrow\; \rho(\mathbf{r})$$

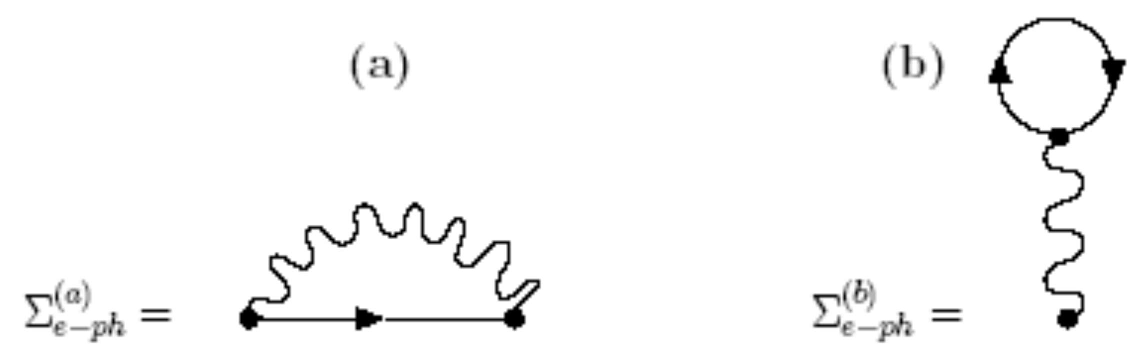
Step 3: Compute electronic Hamiltonian

$$\hat{H}_{\mathrm{K-S}}\,[\,\rho\,] \;=\; \hat{T} \;+\; \hat{V}_{\mathrm{ps}} \;+\; \hat{V}_{\mathrm{H}} \;+\; \hat{V}_{\mathrm{xc}}$$

Step 4: Update Green's function

T. Frederiksen etal, PRL 93, 256601 (2004).

First Born approximation:



Although only 1st order diagrams are included into the phonon self-energy, the SCBA iteration effectively includes higher order diagrams in the sense of RPA.

Theoretical formulation:

e-p self-energies:

$$\Sigma^{\mathrm{R}}_{\mathrm{e-mv}}(E) = \sum_{\nu} g_\nu \, G^{\mathrm{R}}(E - \hbar\,\omega_\nu)\, g^\dagger_\nu + g_\nu \left(G^{<}(E - \hbar\,\omega_\nu) - G^{<}(E + \hbar\,\omega_\nu)\right) g^\dagger_\nu/2$$

$$\Sigma^{<}_{\mathrm{e-mv}}(E) = \sum_{\nu} g_\nu \, G^{<}(E + \hbar\,\omega_\nu)\, g^\dagger_\nu$$

Inelastic correction of the transmission:

$$\delta T(E) = \mathrm{Tr}\,\{\,\Gamma_l(E)\,\Delta A_r(E) \; + \; \Gamma_r(E)\,\Delta A_l(E)\,\}/2$$

Spectral functions:

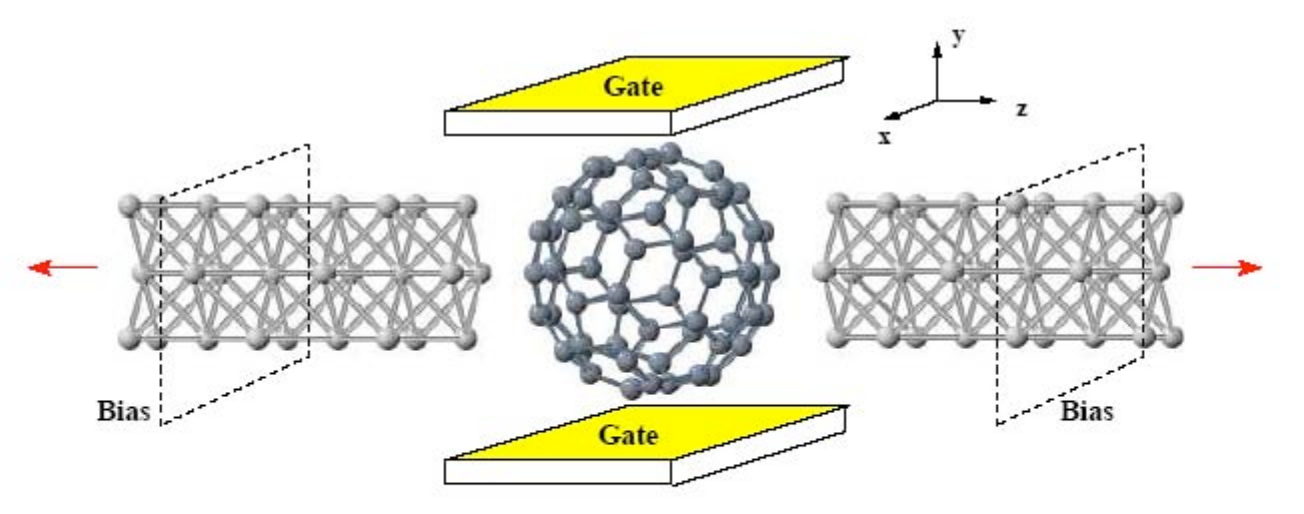
$$\Delta A_l(E) = G^{\mathrm{R}}(E)\,\Gamma_{\mathrm{e-mv},\,l}(E)\,G^{\mathrm{R}\,\dagger}(E) \qquad \Delta A_r(E) = G^{\mathrm{R}}(E)\,\Gamma_{\mathrm{e-mv},\,r}(E)\,G^{\mathrm{R}\,\dagger}(E)$$

The broadening function):

$$\Gamma_{\mathrm{e-mv}}(E) = \sum_{\nu} g_\nu \, A(E - \hbar\,\omega_\nu)\, g^\dagger_\nu + i\, g_\nu \left(G^{<}(E - \hbar\,\omega_\nu) - G^{<}(E + \hbar\,\omega_\nu)\right) g^\dagger_\nu$$

Inelastic correction of the current: $\delta I = (e/h) \int dE\, \delta T(E)\, (n_{\mathrm{F},\,L} - n_{\mathrm{F},\,R})$

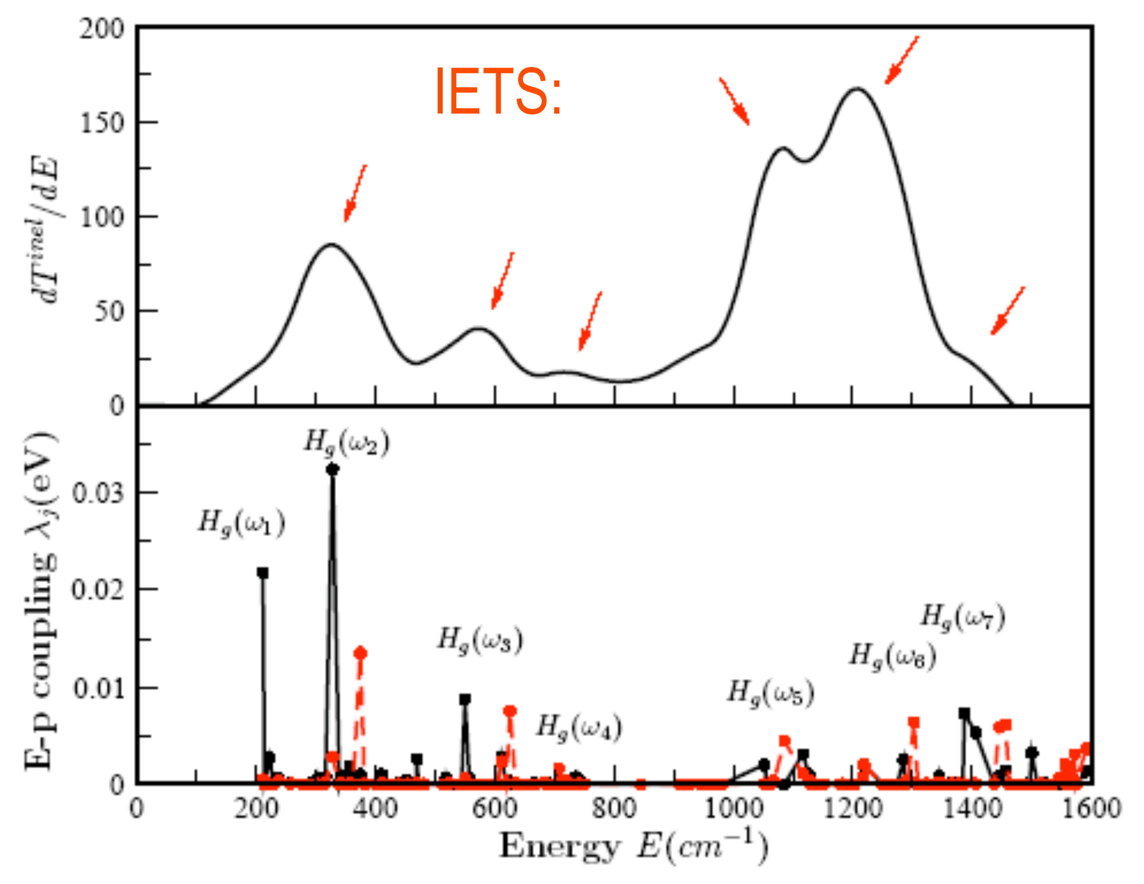
Al-C60-Al MTJ:



1. There are 174 internal vibrational modes, most are highly degenerate. The degeneracy is largely lifted by the leads and bias voltage.
2. Charge transfer of more than 2e from Al leads realigns Fermi level to LUMO of C_{60}, inducing resonance transmission.

Only H_g modes are resolved to be transport active:

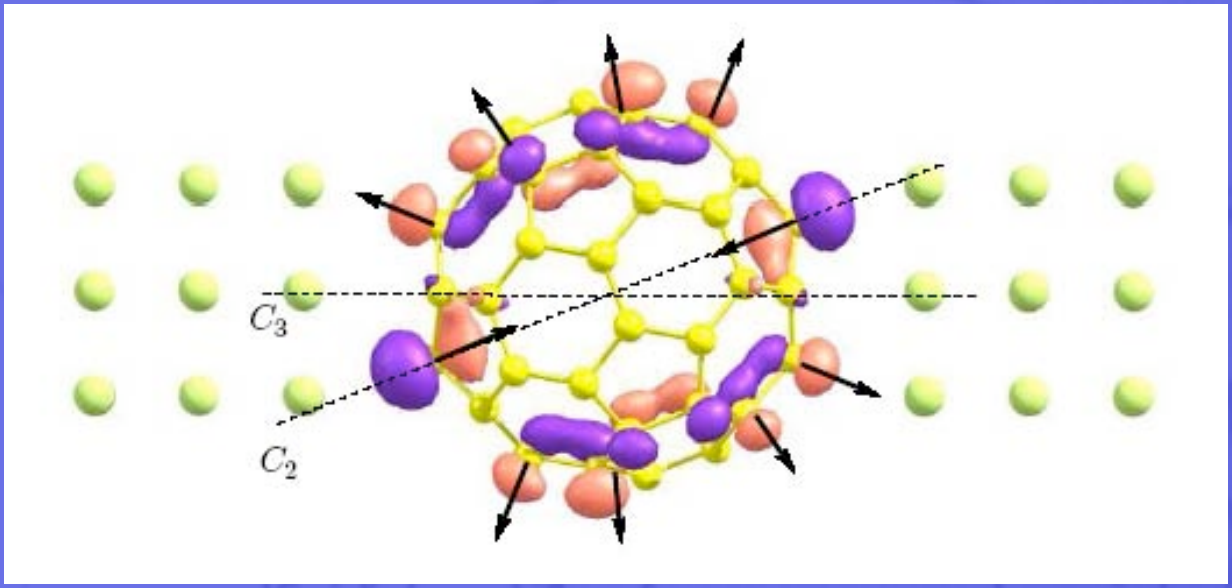
E-p coupling with LUMO



Sergueev, Demkov and Guo, PRB (2007).

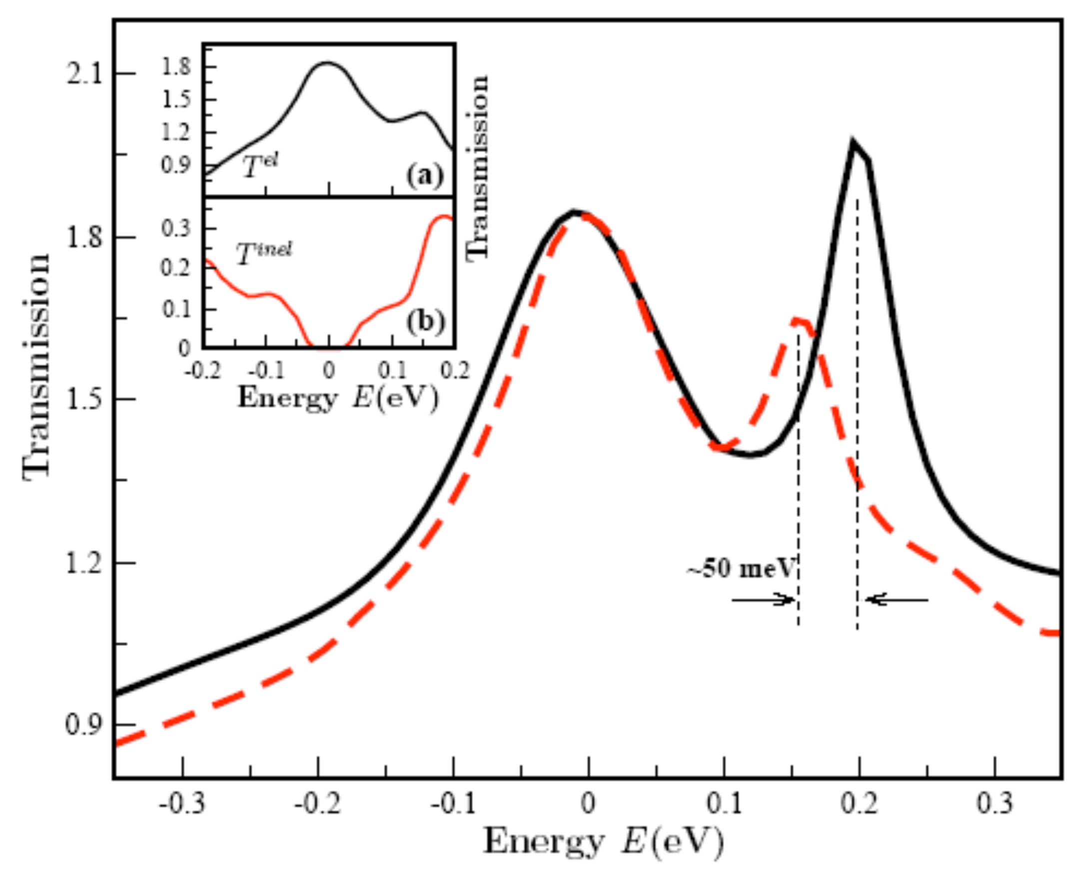
A mode with large effect: $H_g(\omega_1)$

Electron cloud on the LUMO which mediates resonance transmission:



The breathing mode stretches the cage along the C_2 axis so that it changes coupling of C_{60} and the leads. That’s why it has a large effect on transport.

E-p suppresses transport, red-shifts peak:

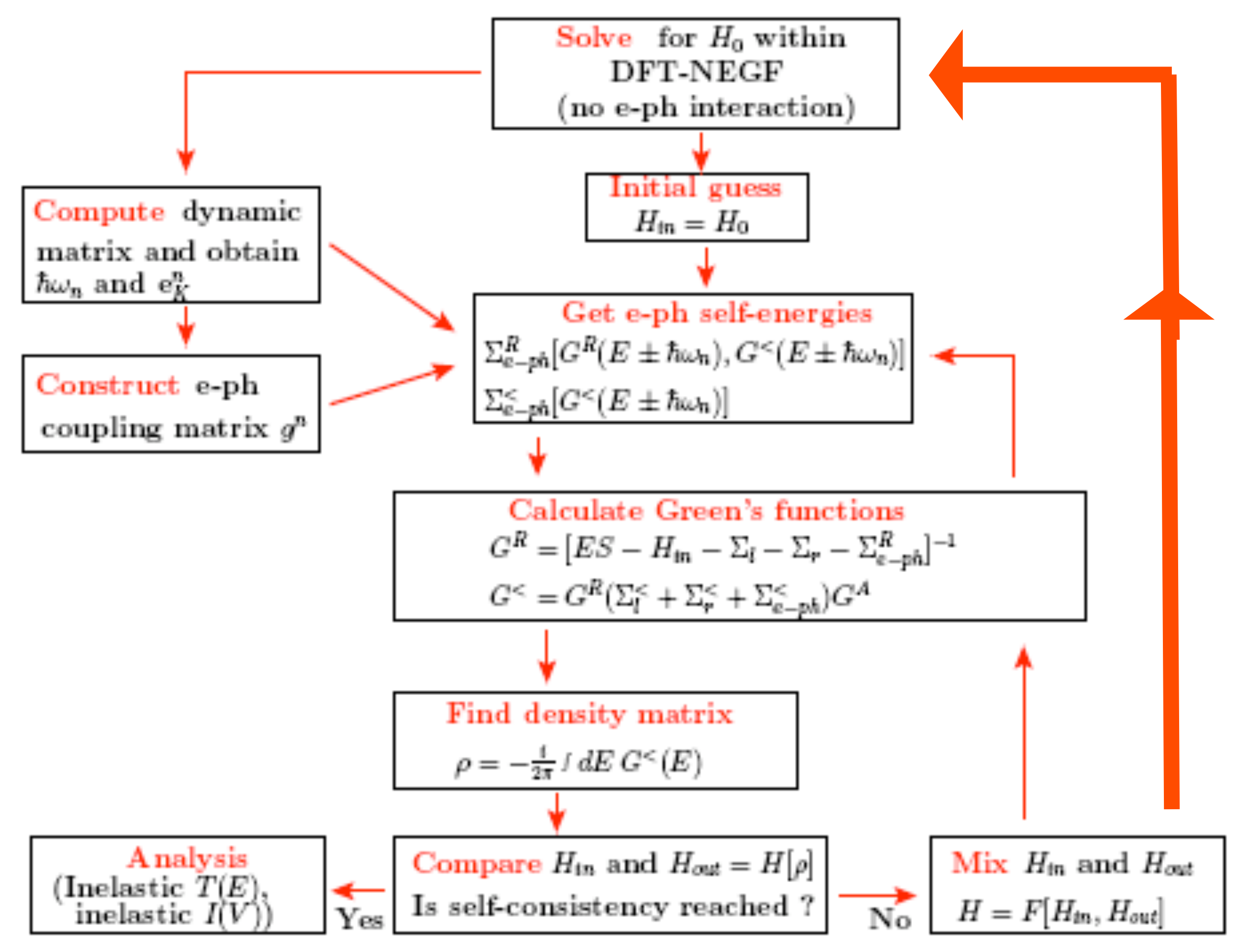


Sergueev, Demkov and Guo (2006).

Lesson learned:

- E-p coupling can depend on non-equilibrium physics during current flow.
- Usually only a few modes are transport active, these tend to affect the transport coupling between the molecule and the leads.
- Difficult to find selection rule for e-p coupling in MTJ.
- For Al-C_{60}-Al MTJ, the resonance LUMO and some of the H_g modes involve the same atoms: resulting to large e-p effect.

Summary of NEGF-DFT-SCBA implementation:



Solve for H_0 within DFT-NEGF (no e-ph interaction)

Initial guess $H_{in} = H_0$

Compute dynamic matrix and obtain $\hbar\omega_n$ and e^n_K

Construct e-ph coupling matrix g^n

Get e-ph self-energies

$\Sigma^R_{e-ph}[G^R(E \pm \hbar\omega_n), G^<(E \pm \hbar\omega_n)]$

$\Sigma^<_{e-ph}[G^<(E \pm \hbar\omega_n)]$

Calculate Green's functions

$$G^R = [ES - H_{in} - \Sigma_l - \Sigma_r - \Sigma^R_{e-ph}]^{-1}$$

$$G^< = G^R(\Sigma^<_l + \Sigma^<_r + \Sigma^<_{e-ph})G^A$$

Find density matrix

$$\rho = -\frac{i}{2\pi} \int dE\, G^<(E)$$

Compare H_{in} and $H_{out} = H[\rho]$
Is self-consistency reached ?

Yes

Analysis
(Inelastic $T(E)$, inelastic $I(V)$)

No

Mix H_{in} and H_{out}
$H = F[H_{in}, H_{out}]$

N. Sergueev, Ph.D thesis, McGill Univ., (2005)

Summary of e-p coupling during current flow:

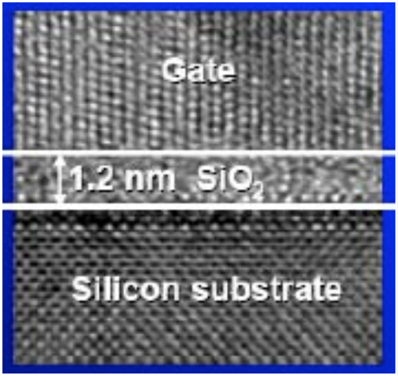
- **Putting a molecule inside a two-probe device changes vibration spectra: low lying modes, frequency changes, selection rule changes.**
- **e-p coupling strength appears to depend on bias voltage, due to participation of additional scattering states as bias is increased. The value of e-p coupling strength also increases with voltage in some system dependent nonlinear way.**
- **It is possible to implement NEGF-DFT-SCBA for analyzing inelastic current, and peaks of correlate roughly with various vibrational modes.**

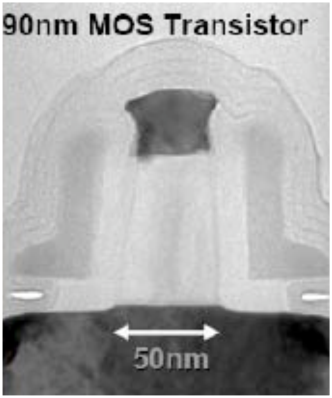
N. Lorente and M. Persson, PRL 85, 2997 (2000). M. J. Montgomery etal. J. Phys.: C 15, 731 (2003). M. Galperin, M. Ratner and A. Nitzan, J. Chem. Phys. 121, 11965 (2004). Y. Asai, Phys. Rev. Lett. 93, 246102 (2004). Y.-C. Chen, M. Zwolak, and M. Di Ventra, Nano Lett. 3, 1691 (2003); ibid 4, 1709 (2004).

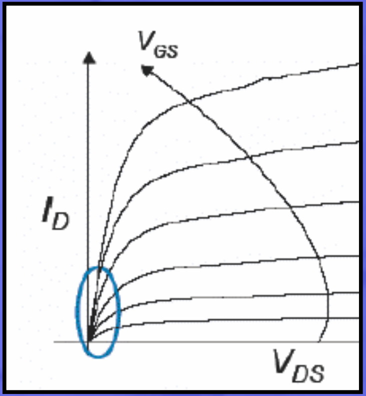
Outline:

- A short review of state-of-the-art;
- DFT atomistic methods;
- The NEGF-DFT implementation;
- Applications of NEGF-DFT;
- Quantum mechanic forces during current flow;
- → Summary: outlook to the near future.

Our goal: atomistic + quantum modeling

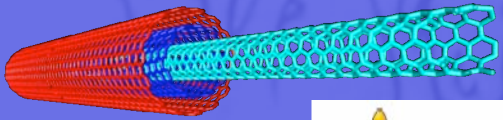


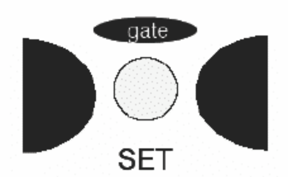


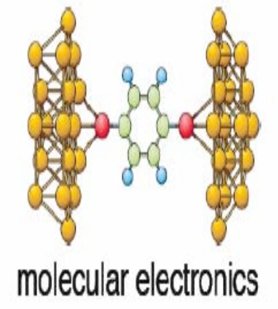


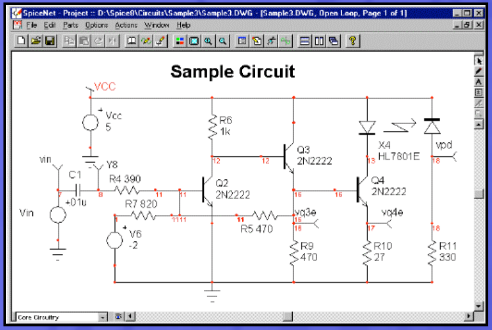
materials,

chemicals,
molecules, ….









atomic quantum modeling software with accuracy

Some summary remarks:

- It appears that NEGF-DFT type formalism has emerged as the main theoretical tool for practical atomistic calculations of molecular electronics. The results are qualitative but can also be quantitative for some situations in comparison with measured data.
- NEGF-DFT type formalism has direct connection to quantum transport theory which is usually done using NEGF (e.g. molecular superconducting tunnel junction).
- It appears that people in NEGF-DFT are moving toward various practical applications of it, and are not working hard enough for its basic theoretical foundation.
- Technical improvements are more often seen (SIC, GW, CI, etc…).
- A potentially fruitful direction is the TDDFT type approach. There are several recent reports for extending TDDFT to open boundary problems so that transport becomes possible. Only a few real calculations exist so far, and even fewer (if at all) compare to measured data. But this is just the beginning and the real outcome is yet to be seen.
- Size limit so far: a few hundred atoms.

Challenging theoretical problems:

1. At single device level, thoroughly understand what works, what does not work, what's the limit, how to improve, on formalisms which are practically calculable. I think NEGF-DFT-type and TDDFT-type are good starting point.

2. How to add more correlations? GW or something drastic like CI ? Computation becomes too complicated will discourage people.

3. Truly far from equilibrium: transients, quantum dissipation etc.

4. Large numbers: how can we go beyond devices with 500 atoms?

5. Solve the Fermi level alignment problem: more experimental data exist now.

6. Solve the contact problem: find better linkers? Switch to semiconductor leads? Also a job for experimentalists.

7. How to efficiently gate a molecular transport junction?

8. Finite temperature effects.

Challenging theory problems (cont.)

- Multiple devices: how to connect them into some thing more interesting? Partially coherent addition of devices?

- Impurities: cannot always do “super-cell” type avrages. Need to develop efficient approaches like CPA, vertex correction, and implement them atomistically and at non-equilibrium level.

- Biomolecules: long history of theory work but seems to be a mess (my lack of knowledge). How to efficiently deal with solvent effects while current is flowing?

- Hybrid systems: transport problems where molecules are interacting with other materials such as superconductors, magnets, etc.

Many further work

Here are two of them:

(i) impurity average

(ii) transient current.

Impurity average:

A new code for impurity averages: NEGF-LMTO-CPA-VC

CPA---coherent potential approximation; VC---vertex correction.

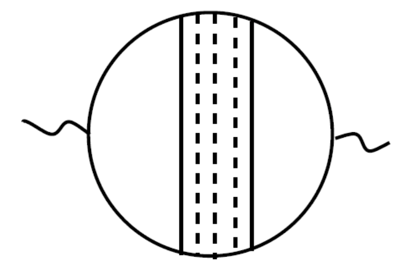
When there are impurities (e.g. Mn doped Ge), we can do two things:

(1) “super-cell” calculations: for each fixed impurity configuration, compute transport; then average over many impurity configurations.

(2) CPA + VC.

$$T(E,\Delta V) = Tr[G^r \Gamma_L G^a \Gamma_R]$$

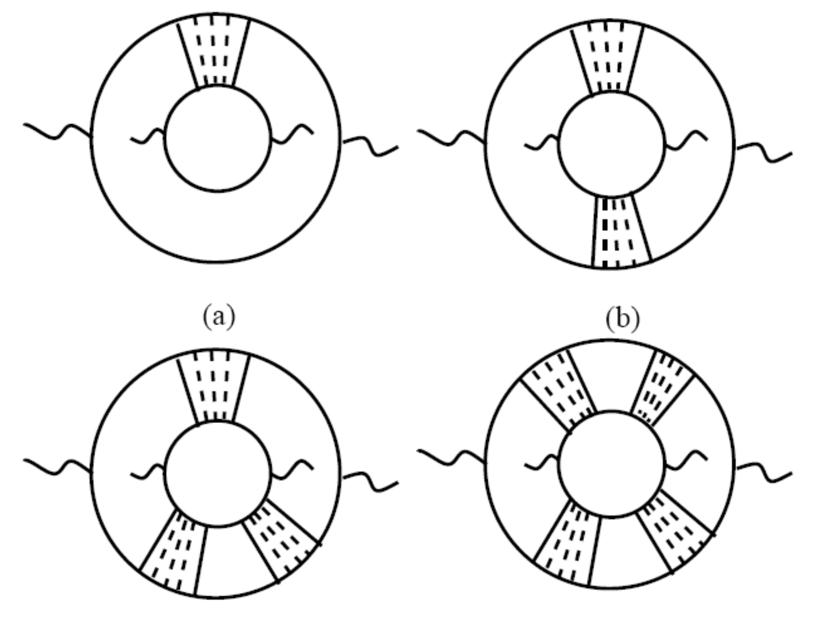
$$G^{\prec} = G^R \Sigma^{\prec} G^A$$



Mahan’s book, p610.

Youqi Ke, K. Xia, HG (2007)

Fluctuations: impurity average over 4 Green’s funcitons

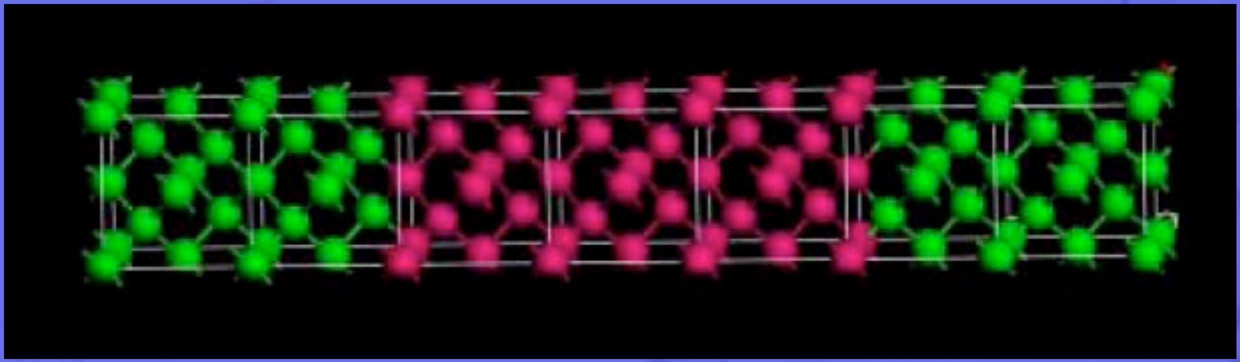


Ning Jia Zhu, HG & R. Harris,
PRL 77, 1825 (1996)

Such calculations can be done, but rather tedious.

With fast computers, we can just grind these diagrams out numerically.

Si-SiMn-Si transport junction:



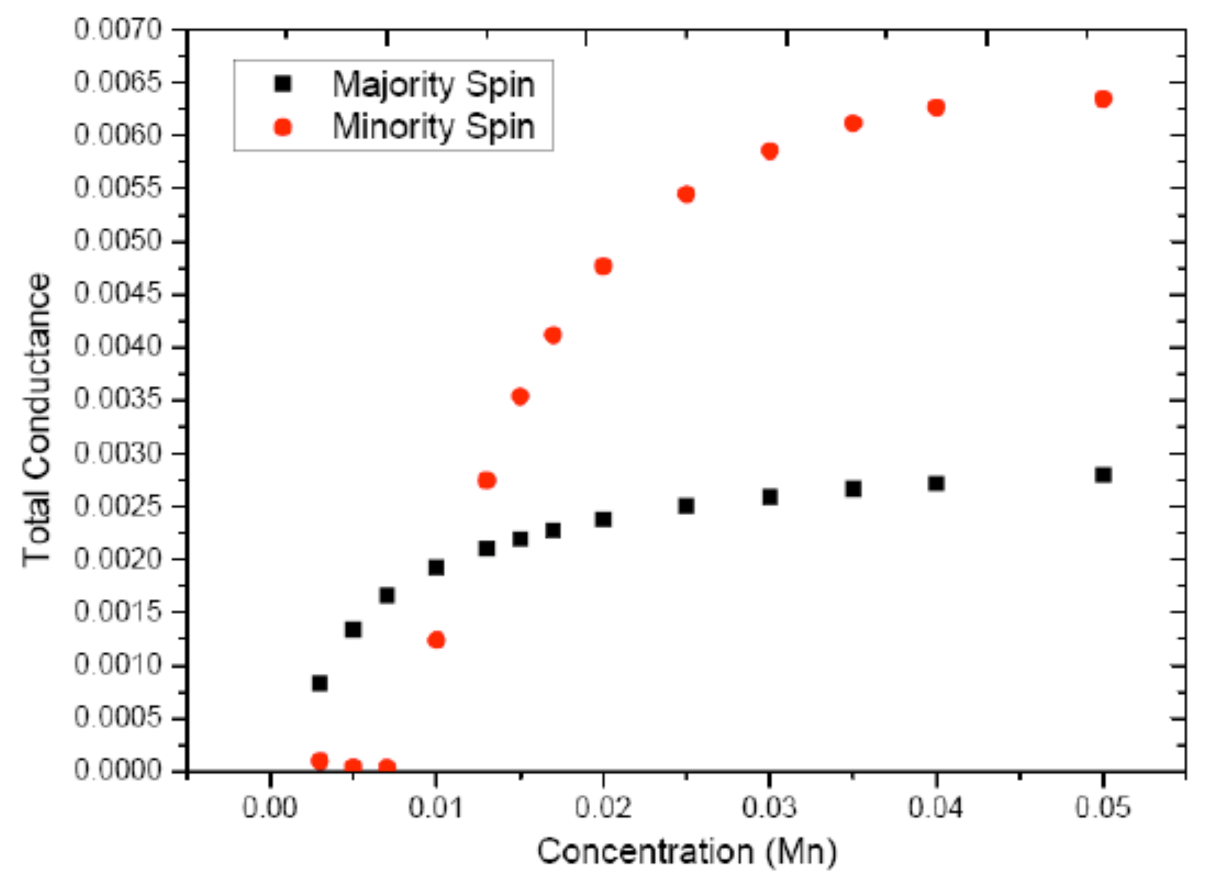
Si leads: heavily doped with P. We use virtual crystal approximation for leads.

Scattering region: Mn doped Si. Atomic structure obtained by WG. Zhu and ZY. Zhang by VASP total energy relaxation.

NEGF-LMTO-CPA-VC for non-equilibrium electronic structure and transport.

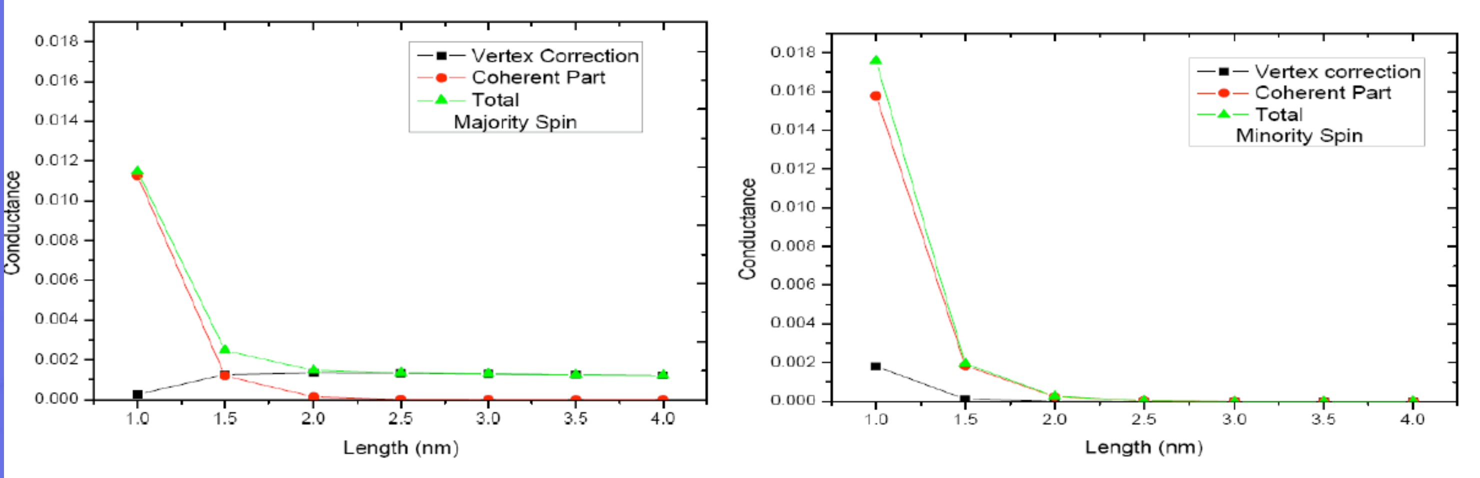
YQ. Ke, WG. Zhu, ZY. Zhang, K. Xia & HG (2007)

Conductance versus Mn content:

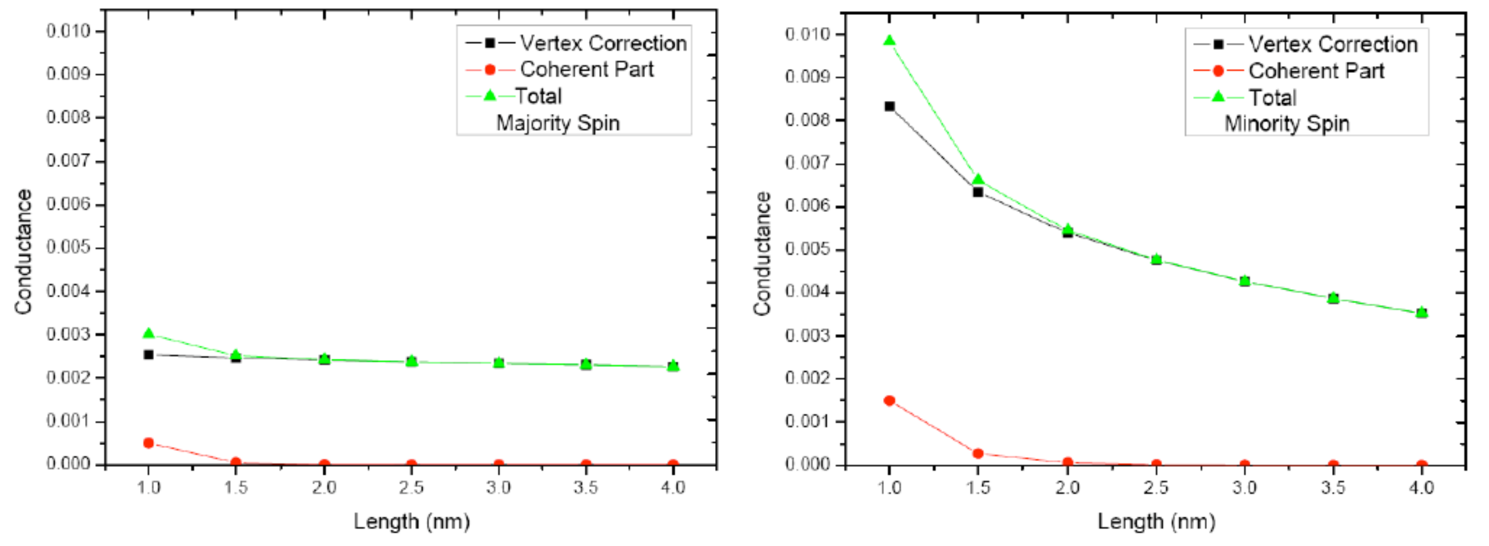


Conductance vs length of SiMn region (preliminary)

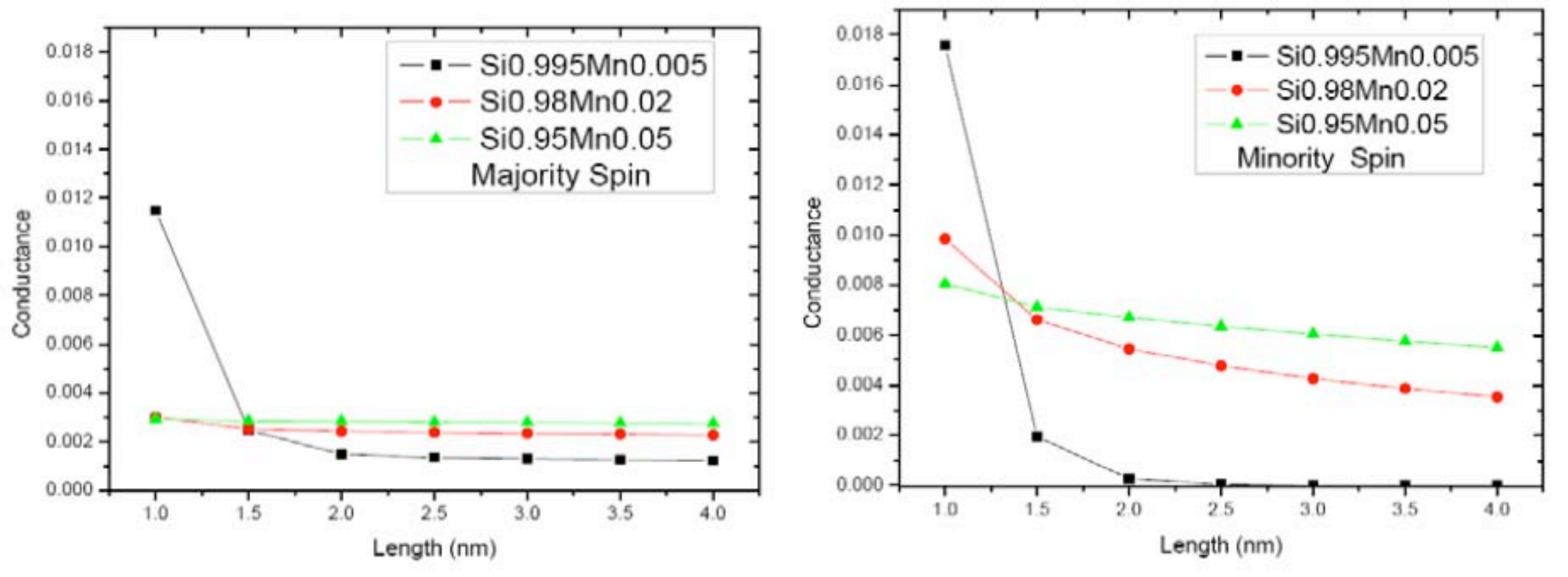
0.5% Mn



2% Mn

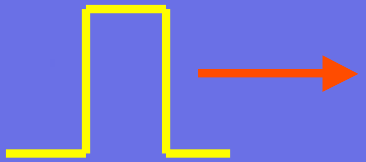


Change Mn doping concentrations:

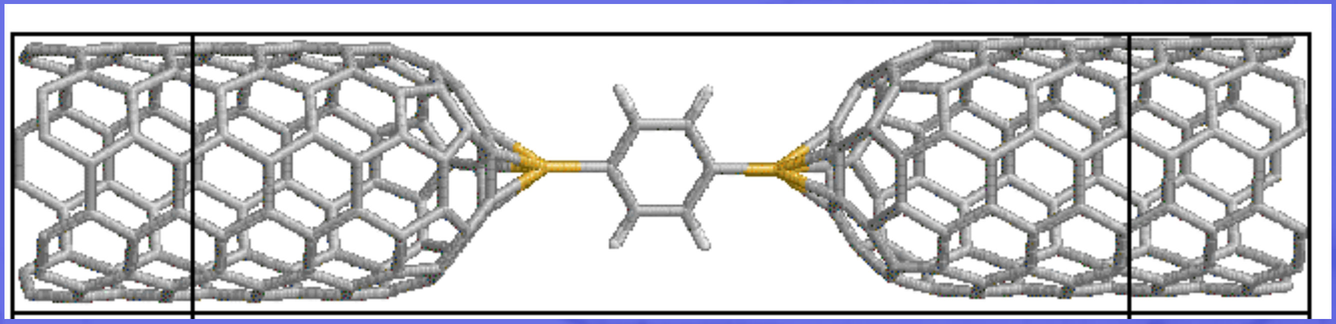


Transient current:

The mixed model: $H = H_{leads} + H_{device} + H_{coupling} + V(t)$



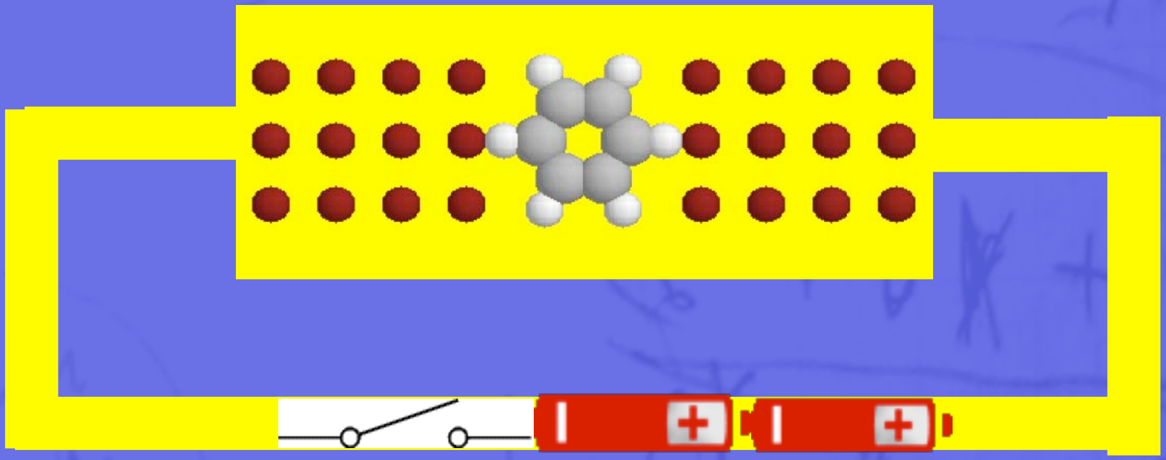
Voltage pulse



1. Include all atomic details: solve $H_0 = H_{leads} + H_{device} + H_{coupling}$ by NEGF-DFT in steady-state, with a partitioned approach;
2. Solve $H = H_0 + V(t)$ by Dyson's equation in a partition free manner;
3. For square shaped pulses, transport described by H can be solved *exactly* including full bandstructures of leads and scattering region.

Maciejko etal PRB 74, 085324 (2006).

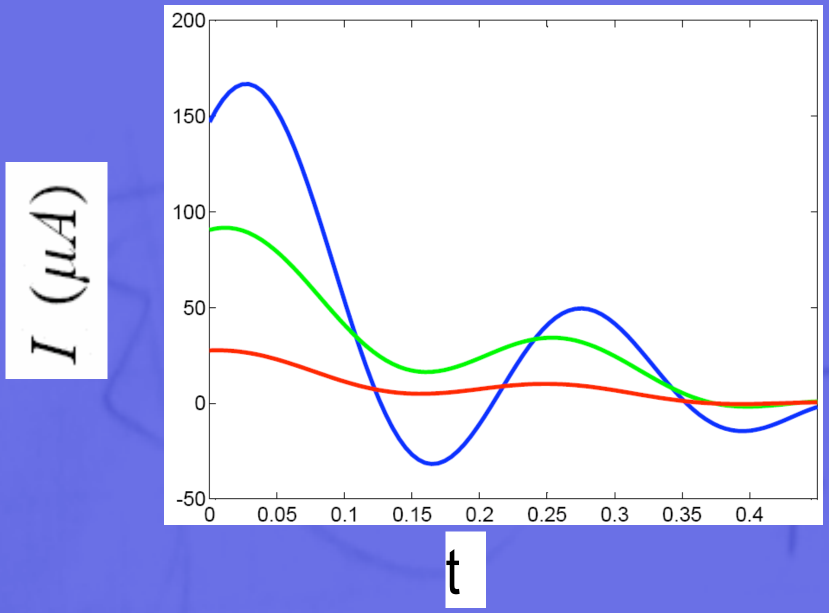
A Molecular Circuit:



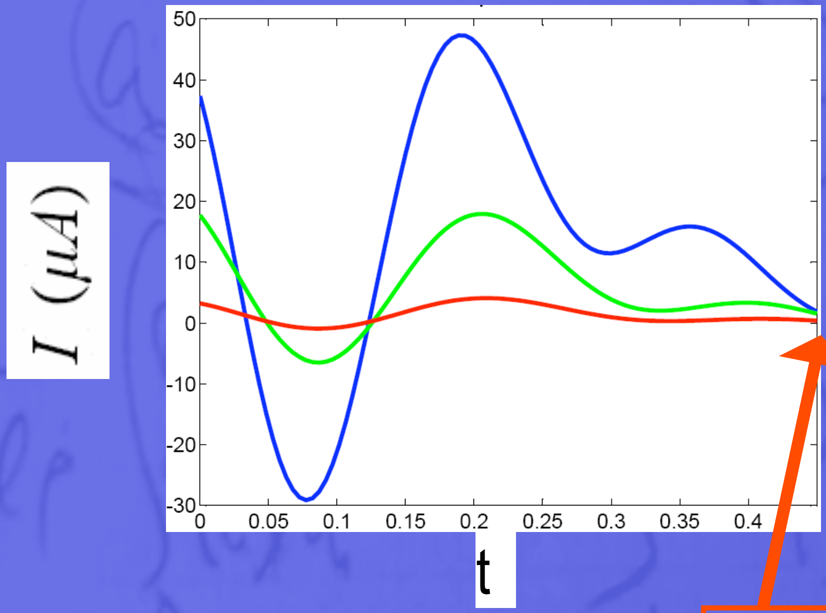
$$I(t) \quad \Leftarrow \quad A_\beta(\epsilon, t) \quad \Leftarrow \int \frac{d\omega}{2\pi}\, e^{-i(\omega-\epsilon)t}\tilde{G}^r(\omega)[\ldots]$$

Analytical properties of $\tilde{G}^r(\omega)$?

Time-dependent Response: from $I(t) \equiv -e\dot{N}(t)$



downward



upward

Steady-state reached.

Pulse height : V = 2.72, 1.36, 0.68 (V)

Nano-electronics: nonequilibrium physics and atomic details

Thank you!

$: NSERC, FQRNT, NanoQuebec, CIFAR, Killam Fellowship Award, SRC, Lu Xin Energy Group.