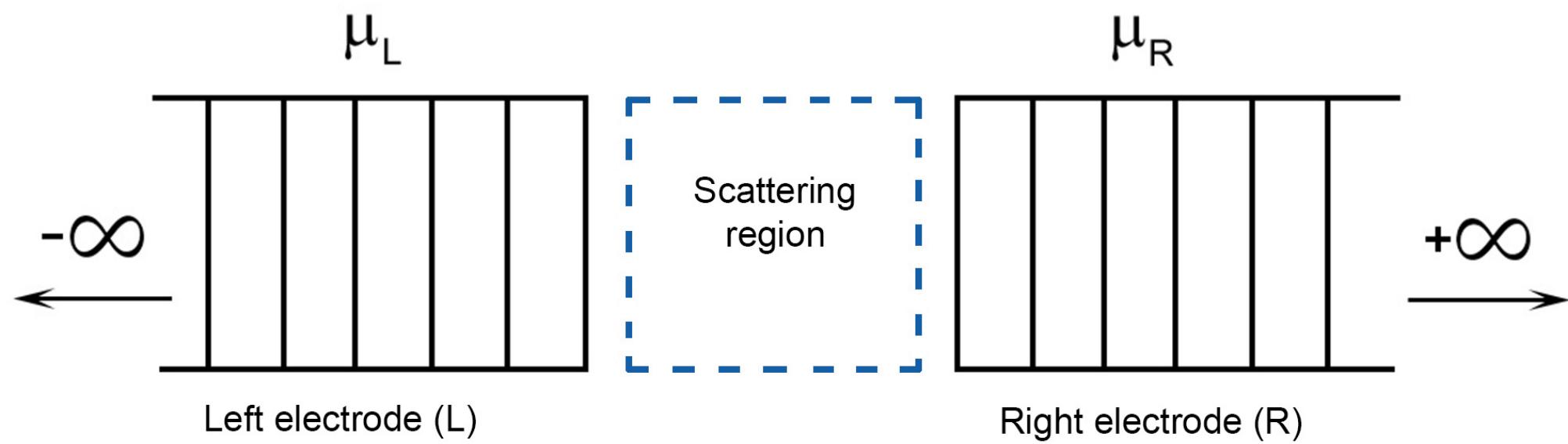


Pedro Brandimarte Mendonça<sup>1</sup>, Alexandre Reily Rocha<sup>2</sup>, Antônio J. R. da Silva<sup>1,3</sup><sup>1</sup> Instituto de Física, Universidade de São Paulo, São Paulo, SP, Brazil<sup>2</sup> Instituto de Física Teórica, Universidade Estadual Paulista Júlio de Mesquita Filho (UNESP), São Paulo, SP, Brazil<sup>3</sup> Laboratório Nacional de Luz Síncrotron, Campinas, SP, Brazil

## MOTIVATION

In this work we present a method that allows one to compute the transport properties of realistic electronic devices with the following features: **large number of randomly distributed defects** together with **realistic electron-phonon interaction**. Our method combines the accuracy and functionality of *ab initio* Density Functional Theory (DFT) to determine the electronic structure and the electron-phonon couplings and vibrational spectra with a recursive Green's functions formalism. We considered the case with weak and localized electron-phonon coupling strength so that the current expression can be expanded to second order in the electron-phonon couplings to obtain recursive expressions for the current. We present results showing the effects produced by considering the electron-phonon interactions in toy models and in graphene nanoribbons with joint attachment of hydroxyl groups.

## METHODOLOGY

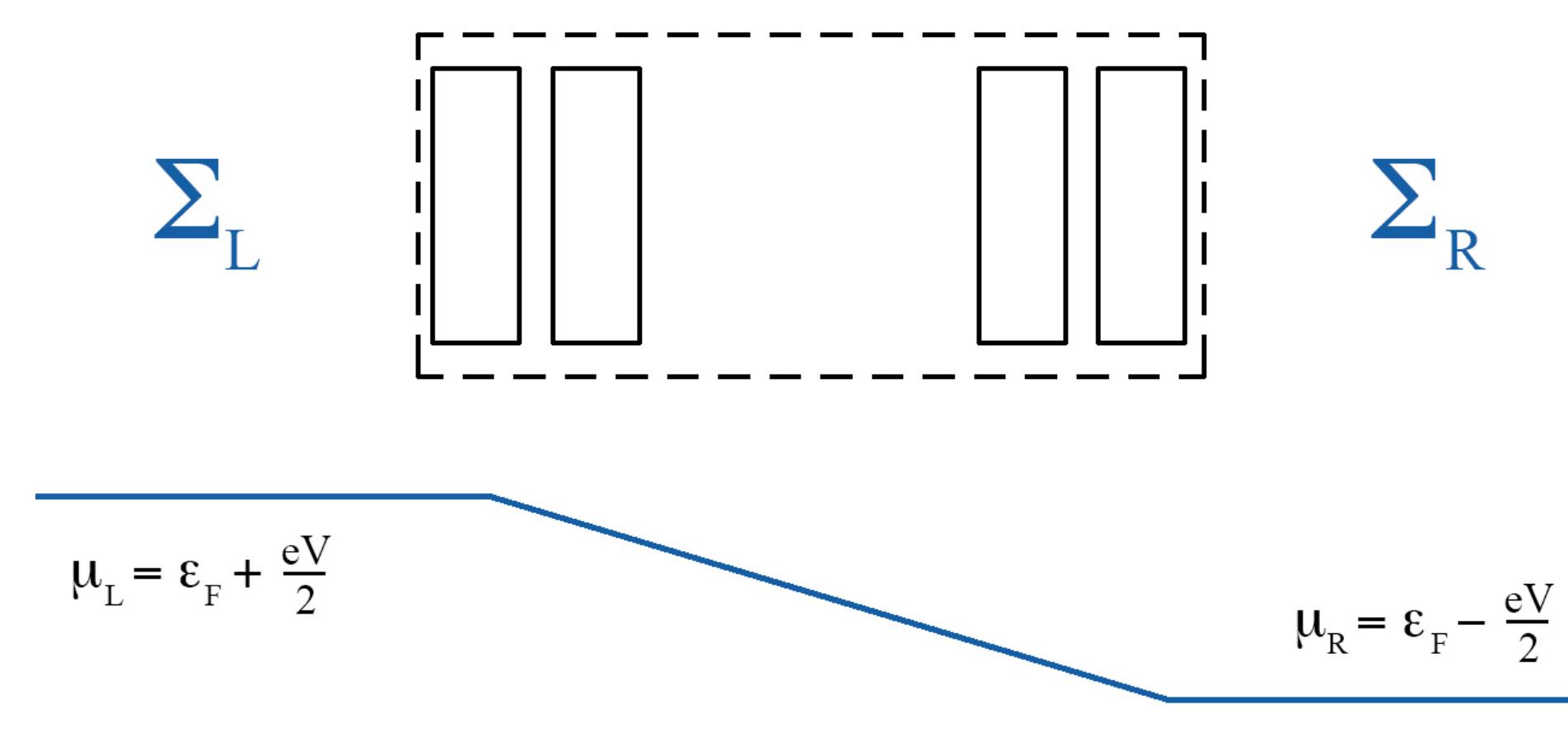


## 1. Elastic Transport (non-interacting systems)

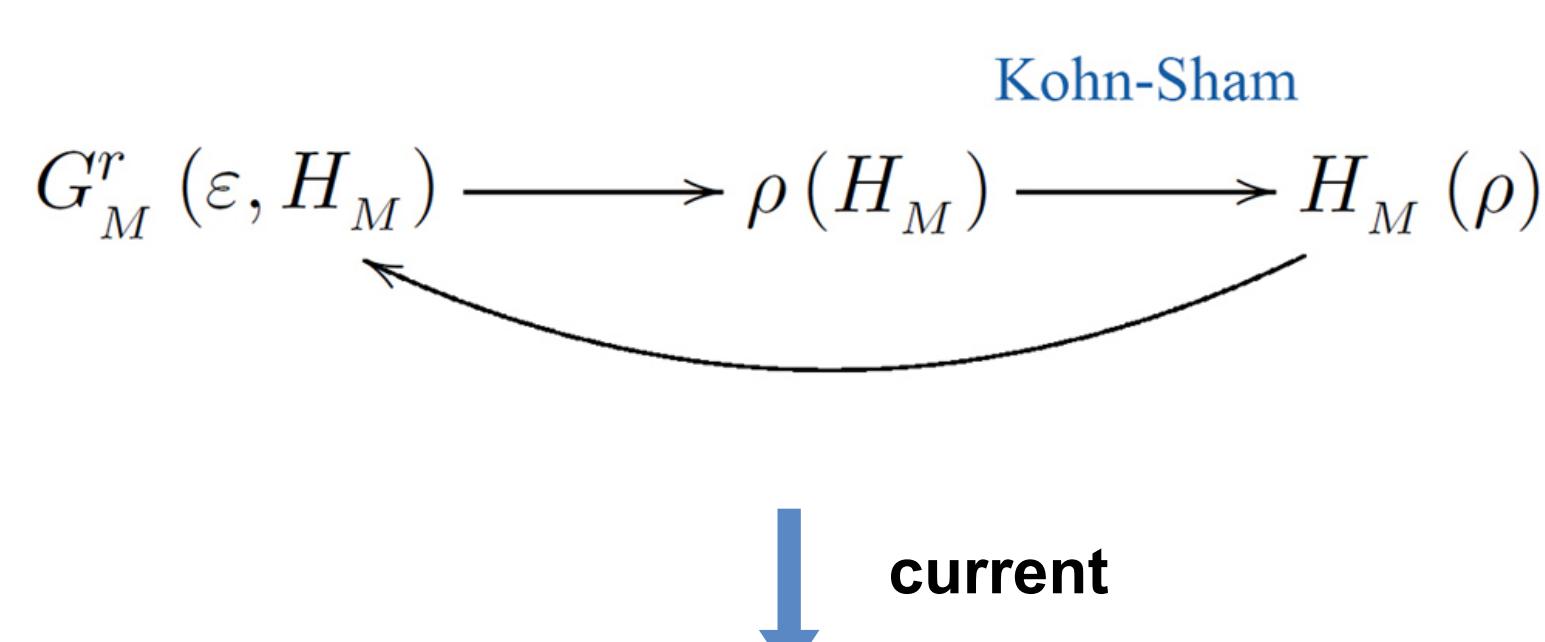
Non-Equilibrium Green's Function formalism (NEGF)

Energy dependent retarded Green's function:

$$[\varepsilon \mathcal{S} - \mathcal{H}] \mathcal{G}^r(E) = \mathbb{1}, \text{ where } \varepsilon = \lim_{\eta \rightarrow 0^+} E + i\eta$$

where  $\mathcal{S}$  and  $\mathcal{H}$  are the overlap and Hamiltonian matrices from the open system.Scattering region ( $M$ ):where  $\Sigma_{L/R}^r$  is the left/right lead self-energy.

SMEAGOL code → density dependent Hamiltonian: DFT + NEGF



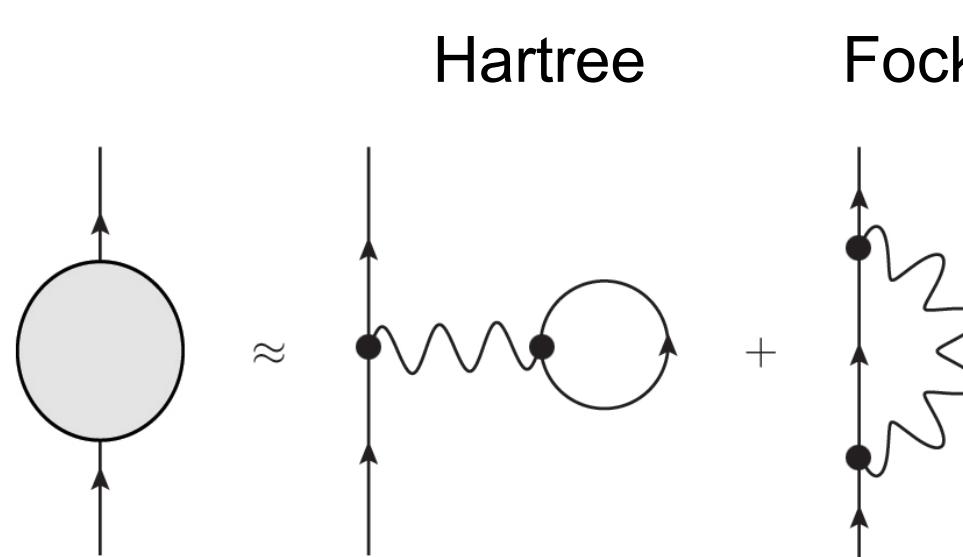
$$I_L = \frac{2e}{h} \int_{-\infty}^{+\infty} d\epsilon \text{Tr} [\Sigma_L^<(\epsilon) G^>(\epsilon) - \Sigma_L^>(\epsilon) G^<(\epsilon)]$$

## 2. Electron-Phonon Interaction

Scattering region coupled to a phonon reservoir in equilibrium:

$$G_M^r = [\varepsilon S_M - H_M - \Sigma_L^r - \Sigma_R^r - \Sigma_{ph}^r]^{-1}$$

## 2.1 Born Approximation (BA)



Feynman rules + Langreth rules for the analytic continuation:

$$\Sigma^{H,r}(\sigma) = i \sum_{\lambda} \sum_{\sigma'} \frac{2}{\hbar \omega_{\lambda}} \int_{-\infty}^{+\infty} \frac{d\epsilon'}{2\pi} M_{\lambda} \text{Tr}[G_0^<(\sigma', \epsilon') M_{\lambda}]$$

$$\Sigma^{F,r}(\sigma, \epsilon) = \frac{1}{2} [\Sigma^{F,>}(\epsilon) - \Sigma^{F,<}(\epsilon)] - \frac{i}{2} \mathcal{H}_{\epsilon'} \{ \Sigma^{F,>}(\epsilon') - \Sigma^{F,<}(\epsilon') \} (\epsilon)$$

where  $\mathcal{H}_{\epsilon'}$  is the Hilbert transform:

$$\mathcal{H}_{\epsilon'} \{ \Sigma^{F,>}(\epsilon') - \Sigma^{F,<}(\epsilon') \} (\epsilon) = \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{+\infty} d\epsilon' \frac{\Sigma^{F,>}(\epsilon') - \Sigma^{F,<}(\epsilon')}{\epsilon' - \epsilon}$$

## 2.2 Lowest Order Expansion

Lowest nontrivial order in perturbation theory with respect to the electron-phonon coupling matrix  $M_{\lambda}$  (i.e.  $O(M_{\lambda}^2)$ ), one can expand the electronic Green's function as  $G^r = G_0^r + G_0^r \Sigma_{ph}^r G_0^r$ .

Applying this expansion on the current equation with BA self-energies and considering the Green's functions and the contact broadening as energy independent (i.e.  $G_0(\epsilon) \approx G_0(\varepsilon_F)$  and  $\Gamma_{L,R}(\epsilon) \approx \Gamma_{L,R}(\varepsilon_F)$ ):

$$\begin{aligned} I^{LOE} \approx & \frac{2e^2}{h} V \text{Tr} [\Gamma_L G_0^r \Gamma_R G_0^r] + \xrightarrow{\text{Büttiker-Landauer}} \text{inelastic terms} \\ & + \sum_{\lambda} \mathcal{I}^{Sym}(V, \hbar \omega_{\lambda}, T, n_{\lambda}) \cdot \\ & \cdot \text{Tr} [G_0^a \Gamma_L G_0^r \left\{ M_{\lambda} G_0^r \Gamma_R G_0^a M_{\lambda} + \frac{i}{2} (\Gamma_R G_0^a M_{\lambda} A_0 M_{\lambda} - \text{h.c.}) \right\}] + \\ & + \sum_{\lambda} \mathcal{I}^{Asym}(V, \hbar \omega_{\lambda}, T) \cdot \\ & \cdot \text{Tr} [G_0^a \Gamma_L G_0^r \left\{ \Gamma_R G_0^a M_{\lambda} G_0^r (\Gamma_R - \Gamma_L) G_0^a M_{\lambda} + \text{h.c.} \right\}] \end{aligned}$$

where

$$\mathcal{I}^{Sym}(V, \hbar \omega_{\lambda}, T, n_{\lambda}) = \frac{2e}{h} \left( 2eV \langle n_{\lambda} \rangle + \frac{\hbar \omega_{\lambda} - eV}{e^{\beta(\hbar \omega_{\lambda} - eV)} - 1} - \frac{\hbar \omega_{\lambda} + eV}{e^{\beta(\hbar \omega_{\lambda} + eV)} - 1} \right)$$

$$\mathcal{I}^{Asym}(V, \hbar \omega_{\lambda}, T) = \frac{e}{h} \int_{-\infty}^{+\infty} d\epsilon [f(\epsilon) - f(\epsilon - eV)] \cdot$$

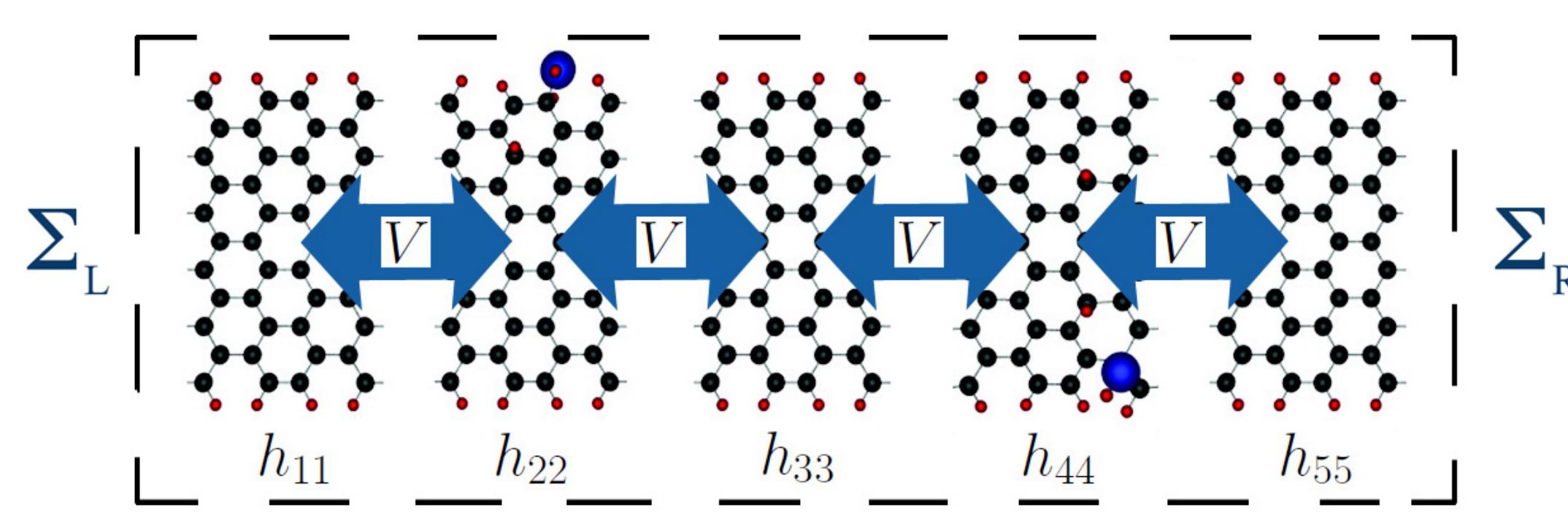
$$\cdot \mathcal{H}_{\epsilon'} \{ f(\epsilon' + \hbar \omega_{\lambda}) - f(\epsilon' - \hbar \omega_{\lambda}) \} (\epsilon)$$

## 3 Electron-Phonon Coupling Matrix

$$M_{ij}^{\lambda} = \sum_{I,\nu} \left\langle i \left| \frac{\partial H_e}{\partial Q_{I\nu}} \right| j \right\rangle_{Q=0} v_{I\nu}^{\lambda} \sqrt{\frac{\hbar}{2M_I \omega_{\lambda}}}$$

## 4 Disordered System

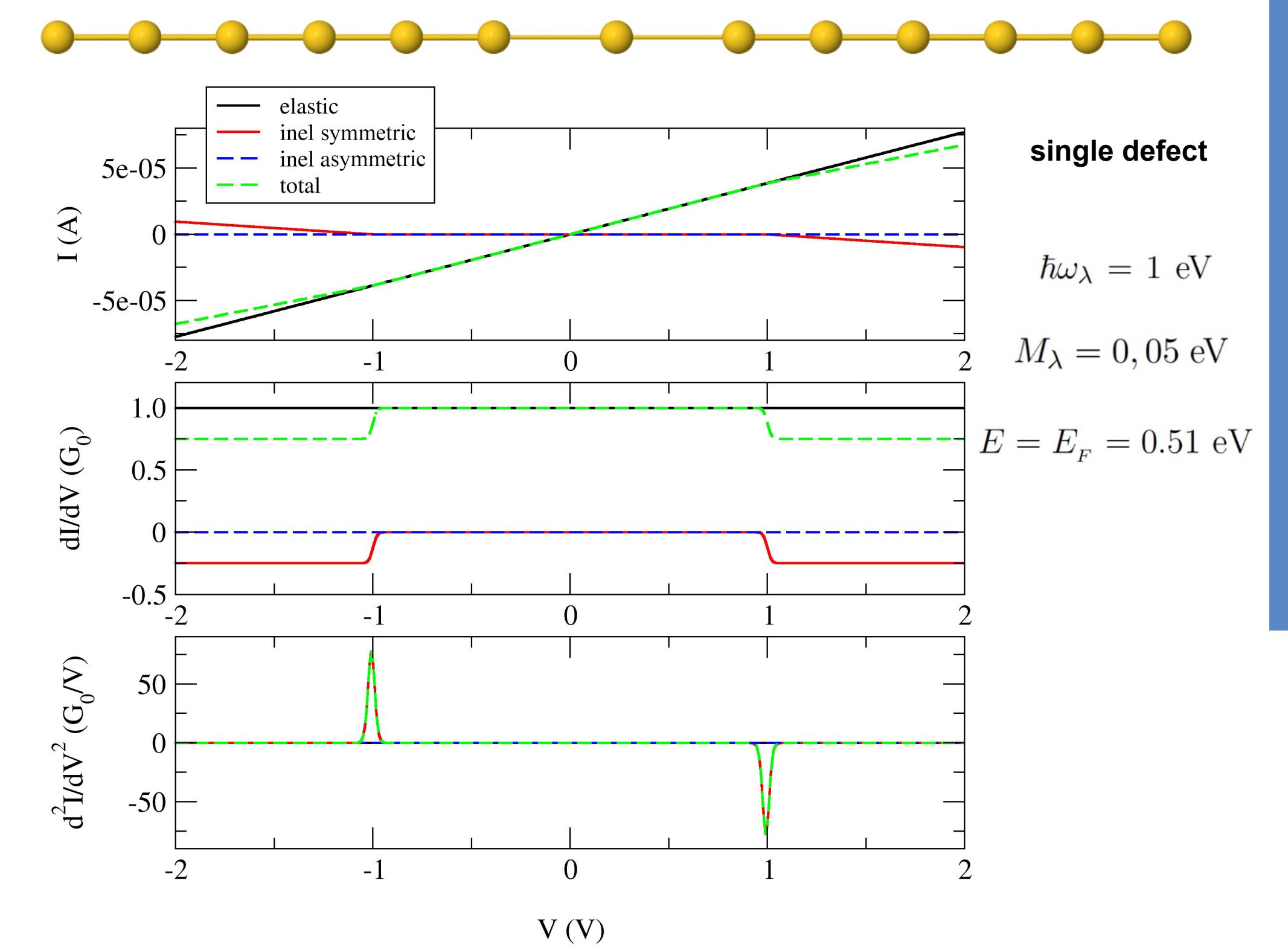
**Recursive Green's function method** to obtain the matrix elements required for LOE expression:



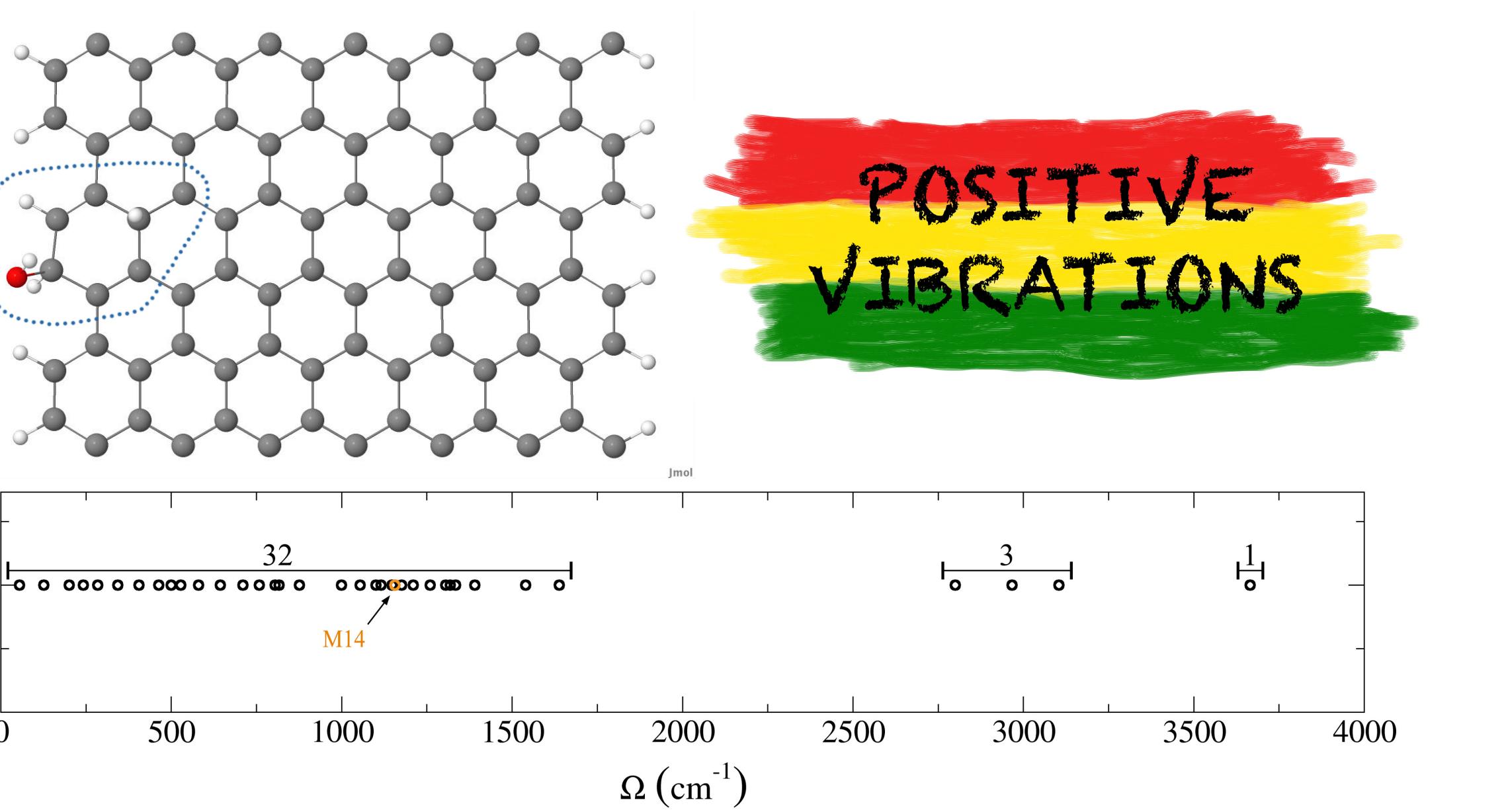
$$\begin{pmatrix} h_{11} & V & 0 & 0 & 0 \\ V^\dagger & h_{22} & V & 0 & 0 \\ 0 & V^\dagger & h_{33} & V & 0 \\ 0 & 0 & V^\dagger & h_{44} & V \\ 0 & 0 & 0 & V^\dagger & h_{55} \end{pmatrix} \begin{pmatrix} G_{11} & G_{12} & G_{13} & G_{14} & G_{15} \\ G_{21} & (G_{22}) & G_{23} & G_{24} & G_{25} \\ G_{31} & G_{32} & G_{33} & G_{34} & G_{35} \\ G_{41} & G_{42} & G_{43} & (G_{44}) & G_{45} \\ G_{51} & G_{52} & G_{53} & (G_{54}) & G_{55} \end{pmatrix} = \mathbb{1}$$

## RESULTS

## 1. One-dimensional Atomic Chain



## 2. Graphene Nanoribbons + Hydroxyl Impurities



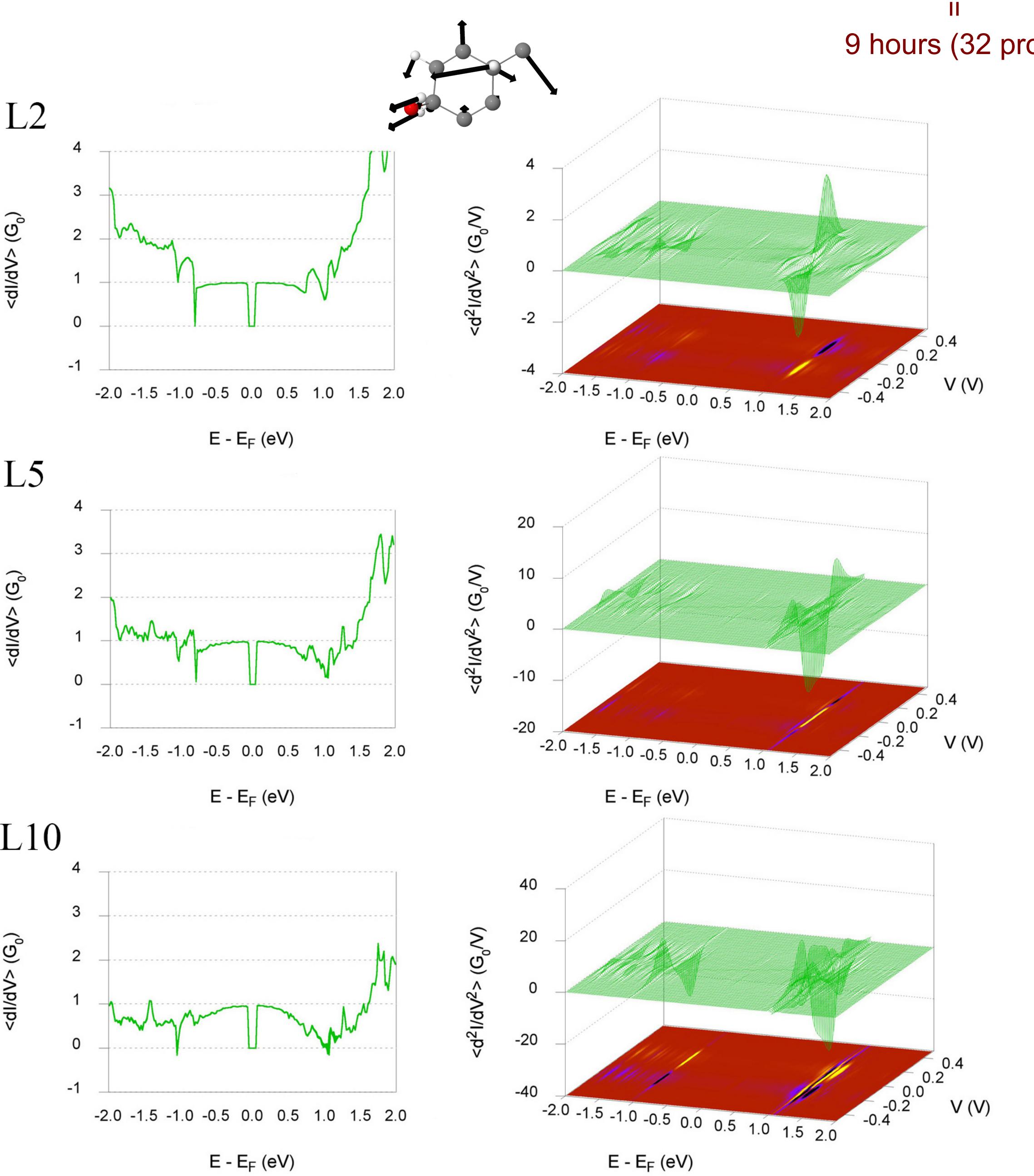
POSITIVE VIBRATIONS

$L_2 = 19,89 \text{ nm} \rightarrow$  blocks: 18 pristine + 2 defects  
 $L_5 = 49,73 \text{ nm} \rightarrow$  blocks: 45 pristine + 5 defects  
 $L_{10} = 99,46 \text{ nm} \rightarrow$  blocks: 90 pristine + 10 defects  
 $L_{20} = 198,92 \text{ nm} \rightarrow$  blocks: 180 pristine + 20 defects

14.780 atoms

177.100 orbitals

9 hours (32 procs)



## ACKNOWLEDGEMENTS