



ICN2^R

Institut Català
de Nanociència
i Nanotecnologia

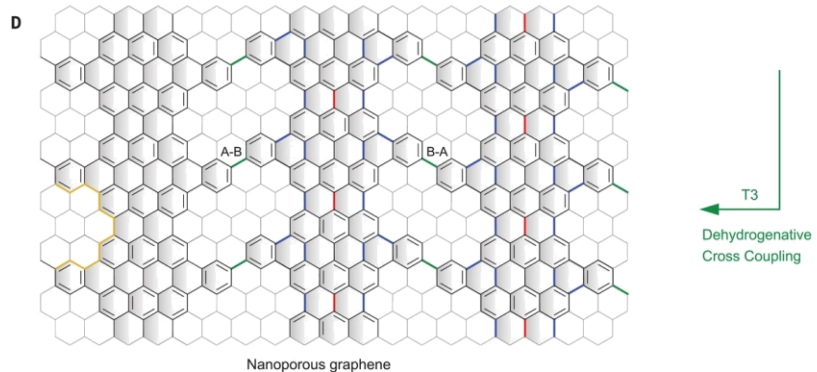
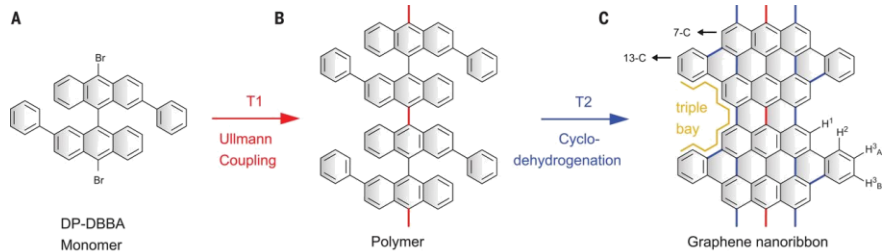
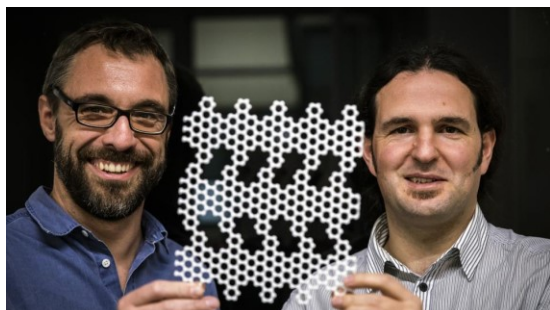
EXCELENCIA
SEVERO
OCHOA

Engineering of Charge Current Flow in Nanoporous Graphenes

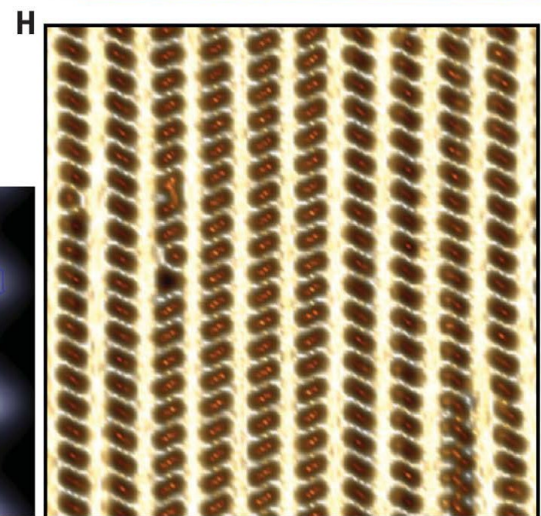
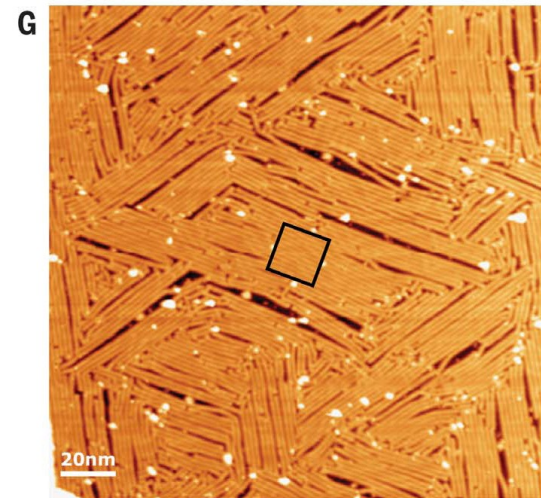
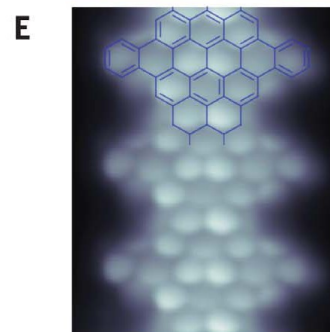
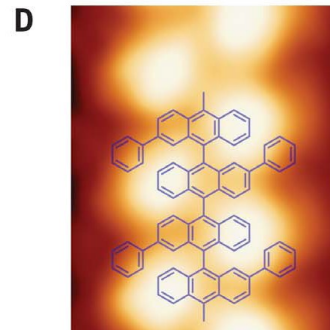
Isaac Alcón – Aron W. Cummings – Stephan Roche



Nanoporous graphenes (NPG)



A. Mugarza, *Science*, 360, 199–203 (2018)



Nanoporous graphene (NPG)

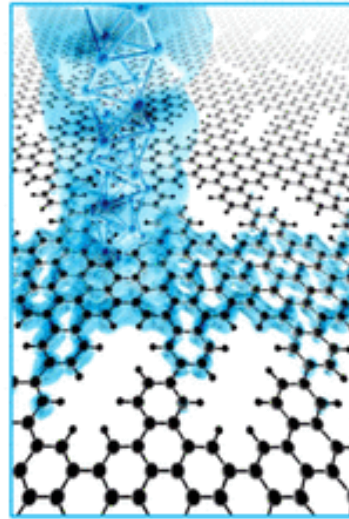


Mads
Brandbyge
DTU Physics

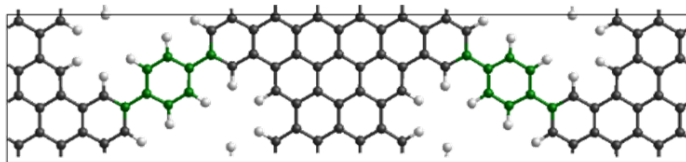
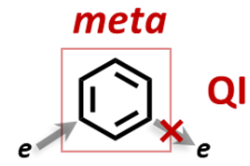
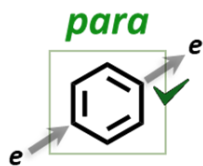
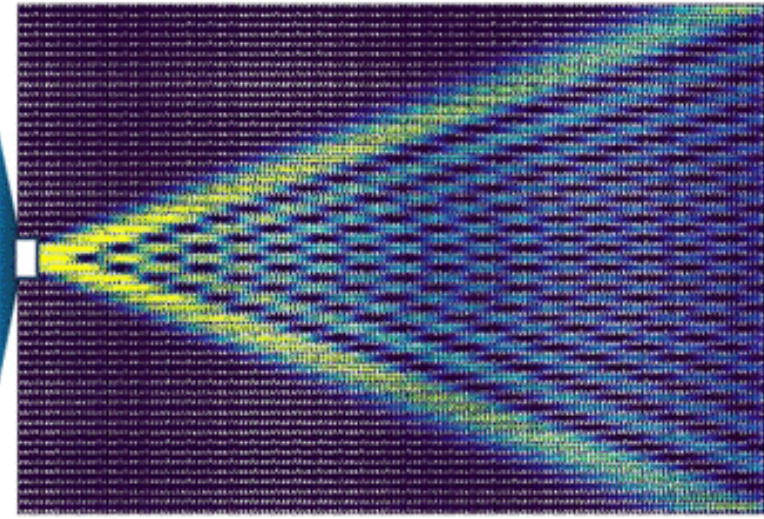
Nano Lett., **2019**, 19, 576–581

NEGF – TranSiesta & TBtrans

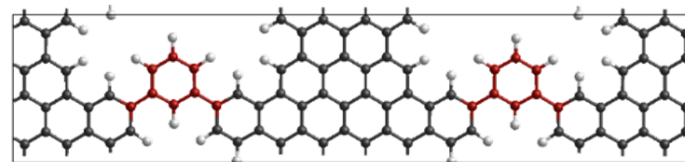
DFT



parametrized TB



para-NPG

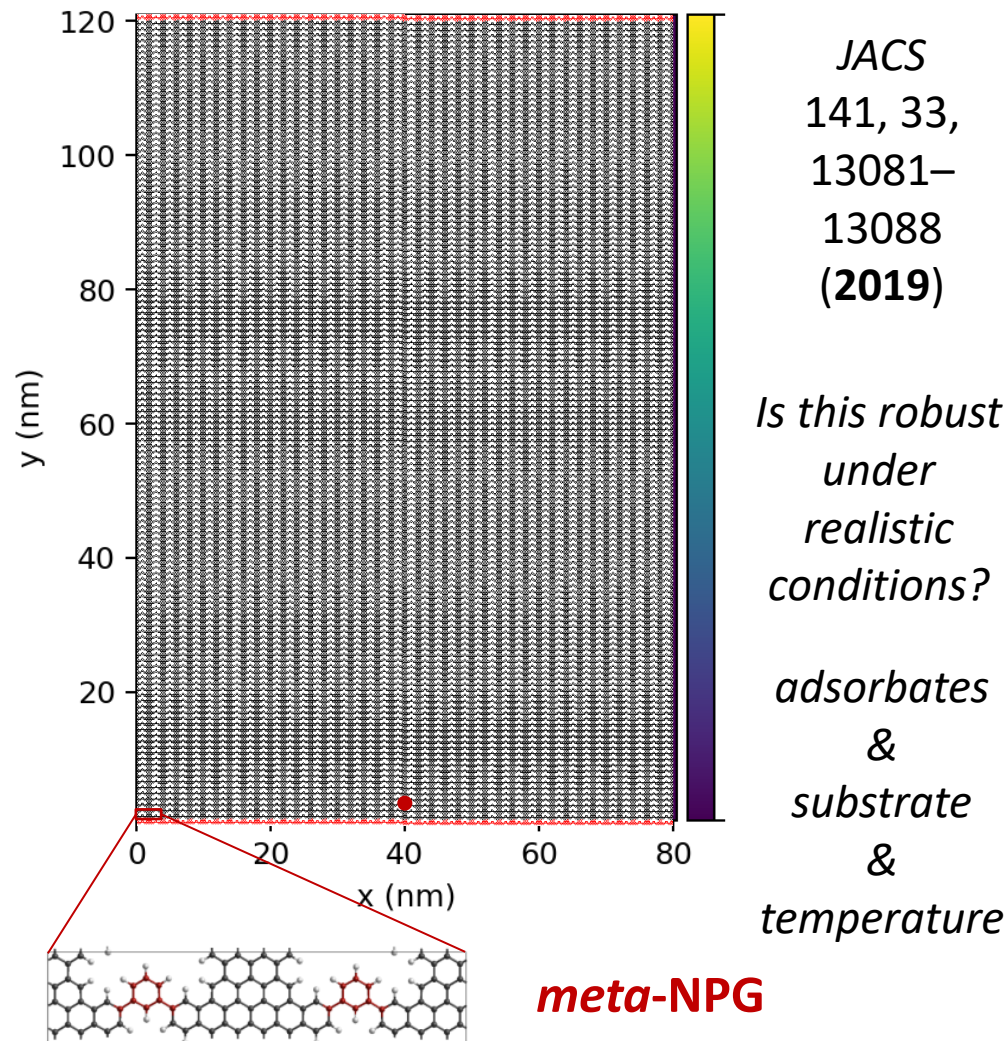
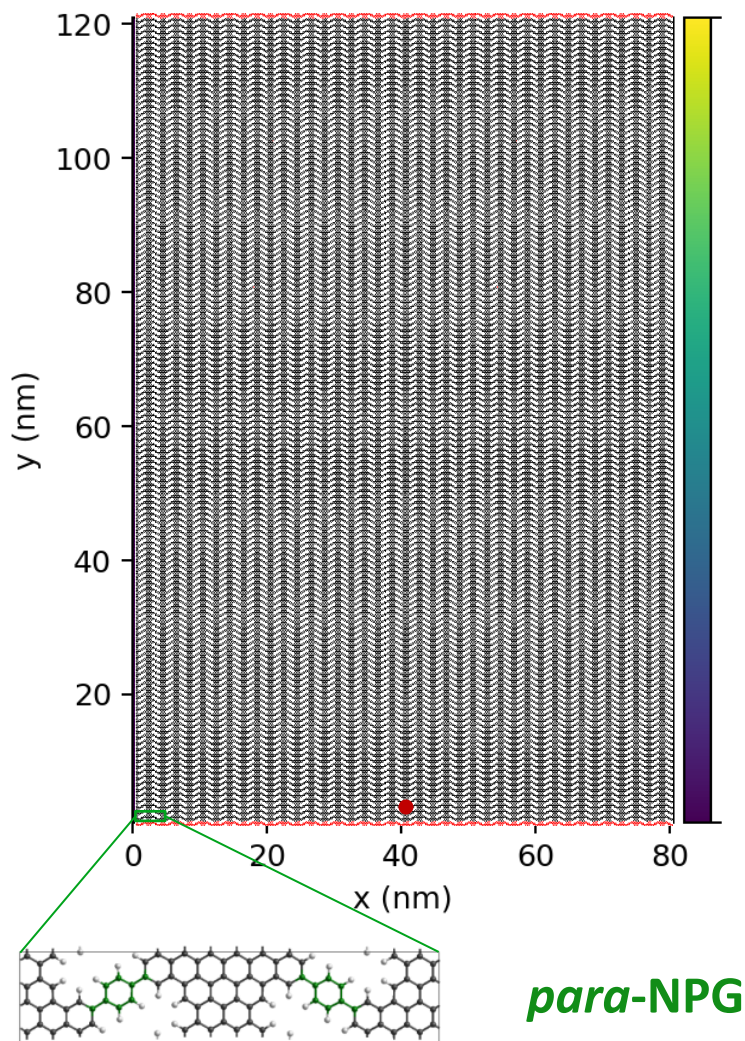


meta-NPG

Quantum interference engineered NPGs: Currents

ca. 250,000 atoms

DFT parametrized TB & NEGF



JACS
141, 33,
13081–
13088
(2019)

*Is this robust
under
realistic
conditions?*

*adsorbates
&
substrate
&
temperature*

LSQT on NPGs: Types of scattering

Thermal fluctuations (finite temperature)

Carbon nanotubes

Phys. Rev. Lett., 2010, 104, 116801

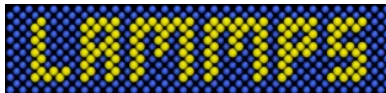


NEGF



LSQT

Molecular Dynamics



Onurcan
Kaya



Aron
Cummings

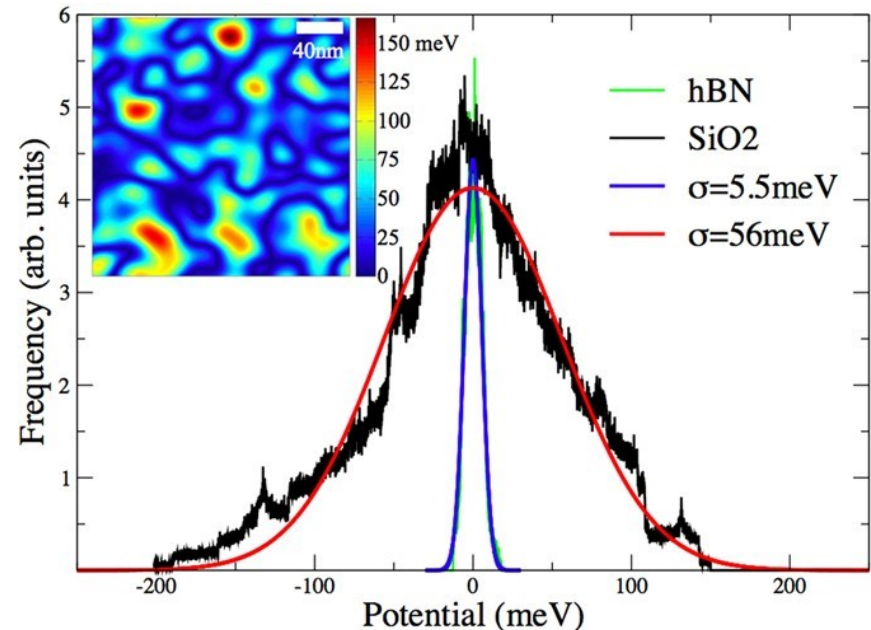
Electrostatic puddles (e.g. substrate effect)

Sci. Rep., 2016, 6, 1–8

Nano Lett., 2017, 17, 5078–5083

Phys. Rev. Lett., 2017, 119, 206601

AIP Adv., 2021, 11, 115007



LSQT: Quantum transport in disordered systems



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Contents lists available at [ScienceDirect](https://www.sciencedirect.com)

Physics Reports

journal homepage: www.elsevier.com/locate/physrep



Linear scaling quantum transport methodologies

Zheyong Fan^{a,b,1}, José H. Garcia^{c,1}, Aron W. Cummings^{c,1},
Jose Eduardo Barrios-Vargas^d, Michel Panhans^{e,f}, Ari Harju^b, Frank Ortmann^{e,f},
Stephan Roche^{c,g,*}

^a School of Mathematics and Physics, Bohai University, Jinzhou, China

^b Varian Medical Systems Finland, Pajukoskenkatu 21, FI-00270 Helsinki, Finland

^c Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and The Barcelona Institute of Science and Technology, Campus UAB, Bellaterra, 08193 Barcelona, Spain

^d Departamento de Física y Química Teórica, Facultad de Química, UNAM, Mexico City 04510, Mexico

^e Center for Advancing Electronics Dresden Technische Universität Dresden 01062 Dresden, Germany

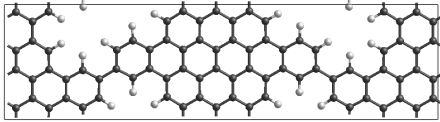
^f Department of Chemistry, Technische Universität München, 85748 Garching, Germany

^g ICREA – Institució Catalana de Recerca i Estudis Avançats, 08010 Barcelona, Spain

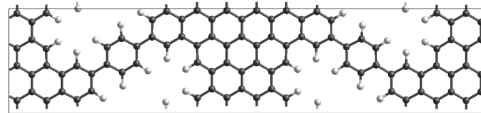
Fan, Z. *et al.* Linear scaling quantum transport methodologies. *Physics Reports*
903, 1–69 (2021)

Nanoporous graphenes (NPGs)

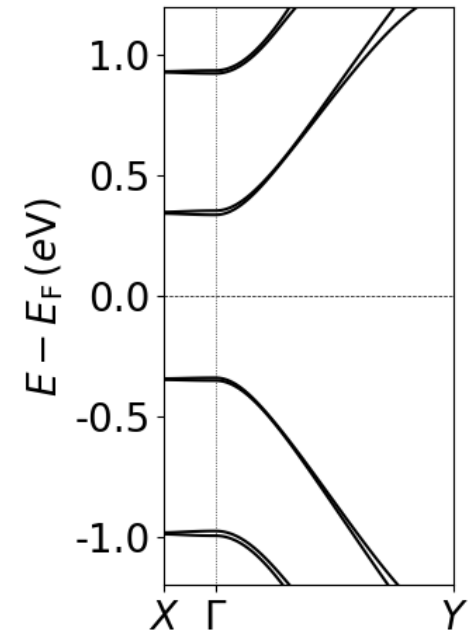
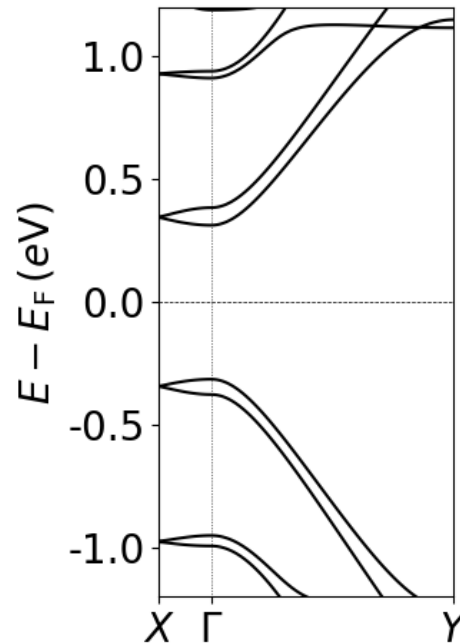
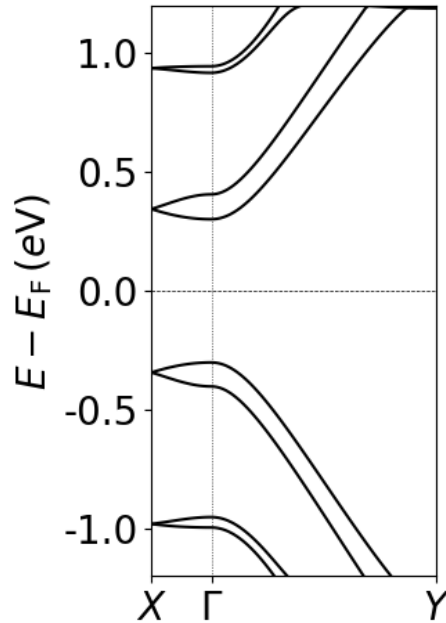
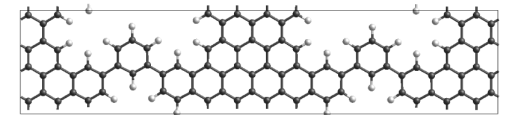
fNPG



para-NPG



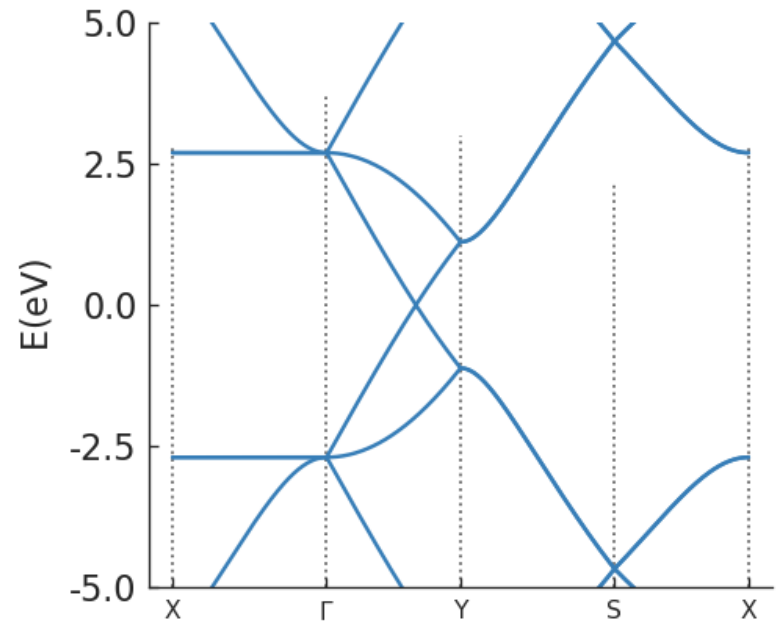
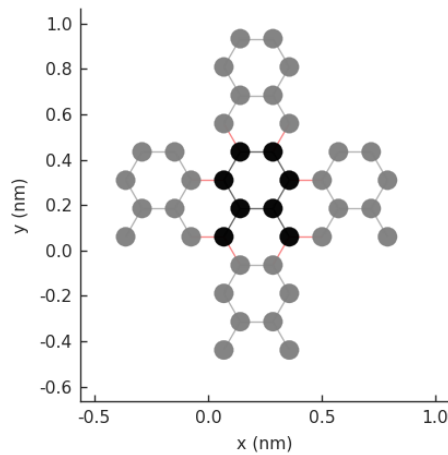
meta-NPG



DFT (PBE; Siesta)

Nanoporous graphenes (NPGs)

graphene

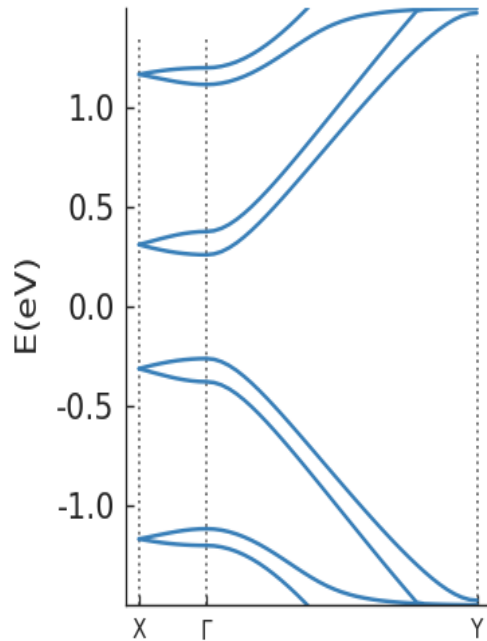
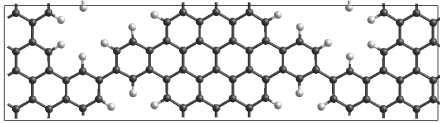


Pybinding

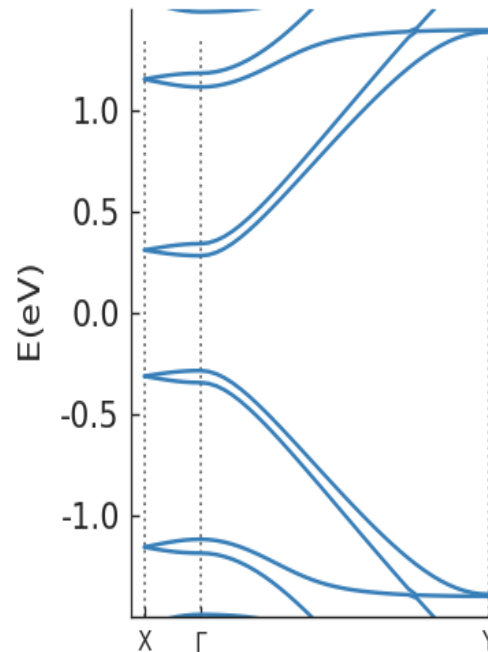
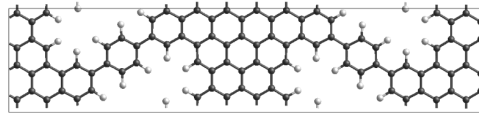
1st nn TB p_z effective Hamiltonian

Nanoporous graphenes (NPGs)

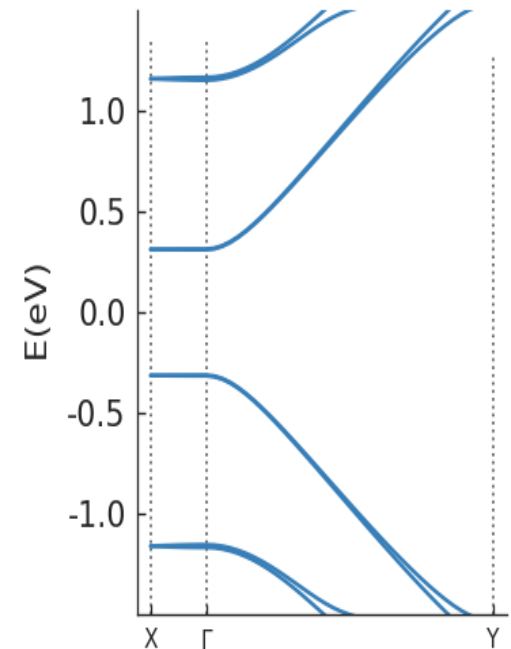
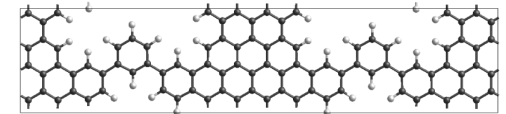
fNPG



para-NPG



meta-NPG



1st nn TB p_z effective Hamiltonian

Disordered systems – Electrostatic puddles

$$\varepsilon_i^{\text{new}} = \varepsilon_i^0 + W \cdot e^{-\frac{1}{2} \frac{D^2}{\sigma^2}} \left\{ \begin{array}{l} W [-2.8, +2.8] \text{ eV} \\ D \rightarrow \text{distance to the puddle center} \\ \sigma = 4.35 \text{ \AA} (\approx 3 \cdot a_{cc}) \rightarrow \text{puddle width} \end{array} \right.$$

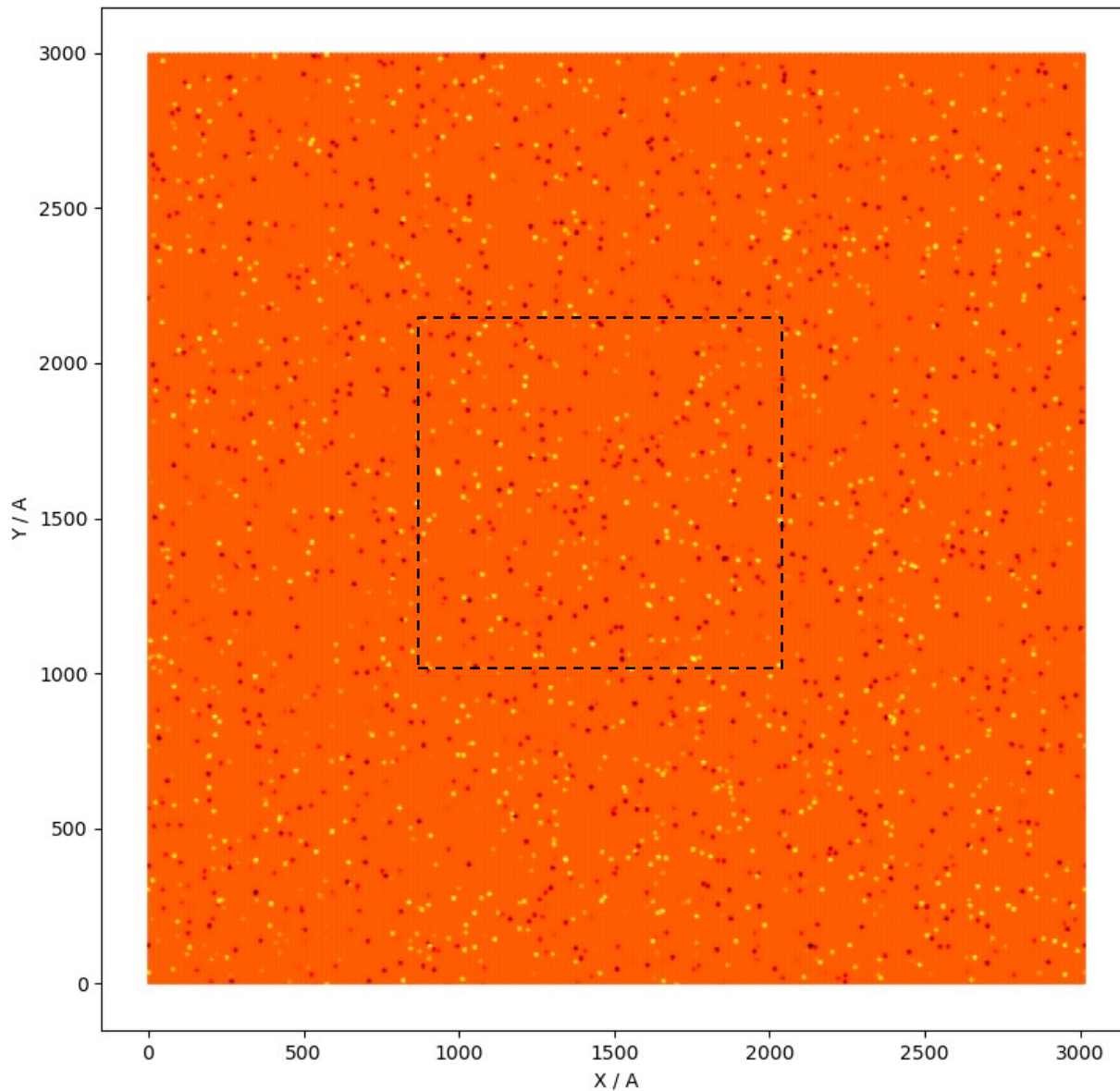
$$C_{\text{puddles}} = 0.1\%$$

$$\text{cutoff} = 6\sigma \approx 26.1 \text{ \AA} \rightarrow \Delta\varepsilon > 4 \cdot 10^{-8} \text{ eV}$$

300 x 300 nm² samples

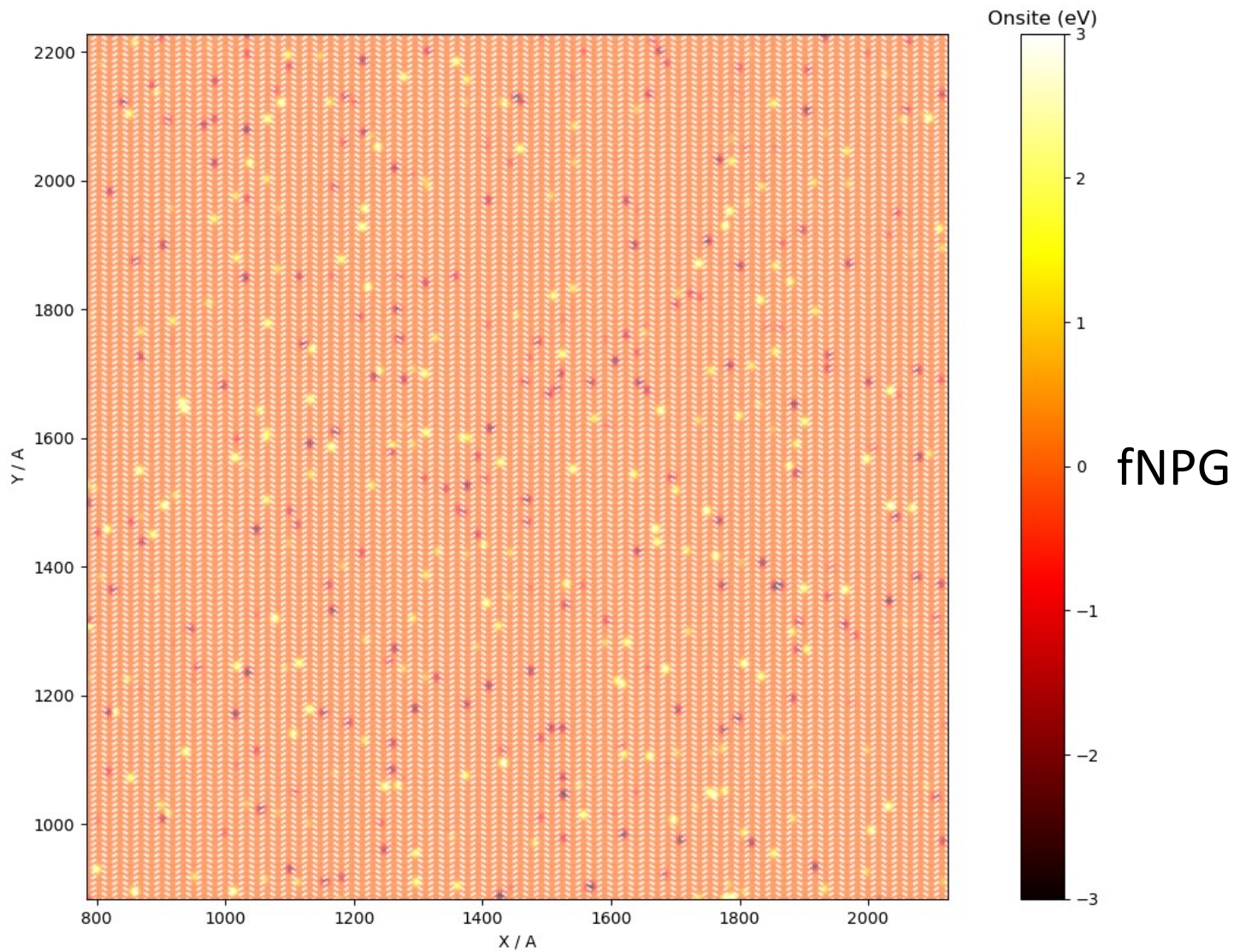
	$V_x [\text{\AA}]$	$V_y [\text{\AA}]$	$t \cdot \text{los} (x/y)$	$\mu_0 \text{ at}$
Gr	3006	2993	174/200	3.340.800
NPG	3016	2999	92/345	2.539.200
P NPG	3019	2999	75/345	2.380.500
w NPG	3019	2999	75/345	2.380.500

Disordered systems – Electrostatic puddles



fNPG

Disordered systems – Electrostatic puddles



LSQT Setup

LSQT parameters

DOS: $\eta = 0.02$ eV (20 meV)

Time-step = 10 fs

Varying # time-steps (4 ps – 32 ps)

$$E_F = 0.4 \text{ eV}$$

Propagation length

$$L_x = \sqrt{\Delta X^2(E, t)}$$

Diffusion coefficient

$$D_x(E, t) = \frac{1}{2} \frac{d\Delta X^2(E, t)}{dt}$$

Conductivity

$$\sigma_x(E, t) = D_x(E, t) \cdot \rho(E) \cdot e^2$$



Statistics

4 materials

5 puddle distributions per mat.

10 random phases per distr.

Propagation length

$$L_y = \sqrt{\Delta Y^2(E, t)}$$

Diffusion coefficient

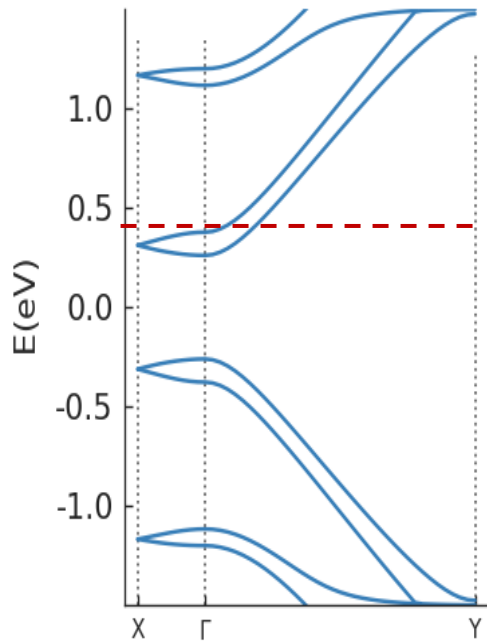
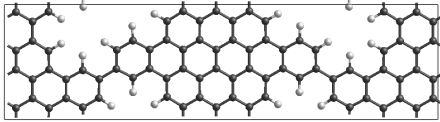
$$D_y(E, t) = \frac{1}{2} \frac{d\Delta Y^2(E, t)}{dt}$$

Conductivity

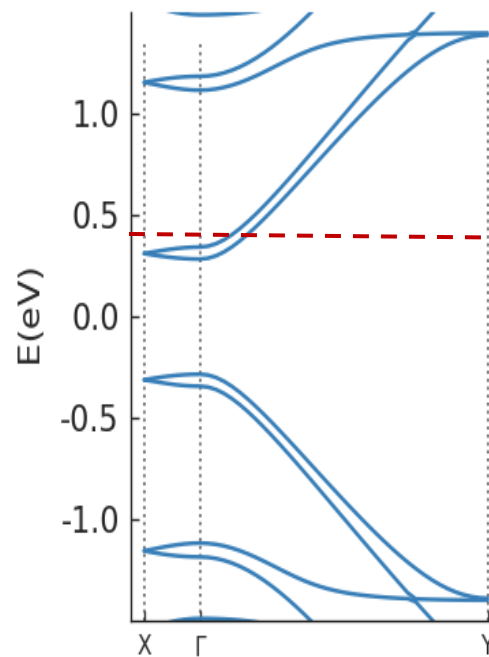
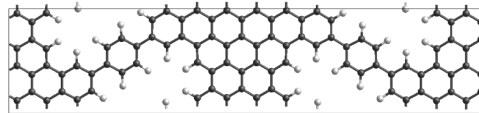
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Nanoporous graphenes (NPGs)

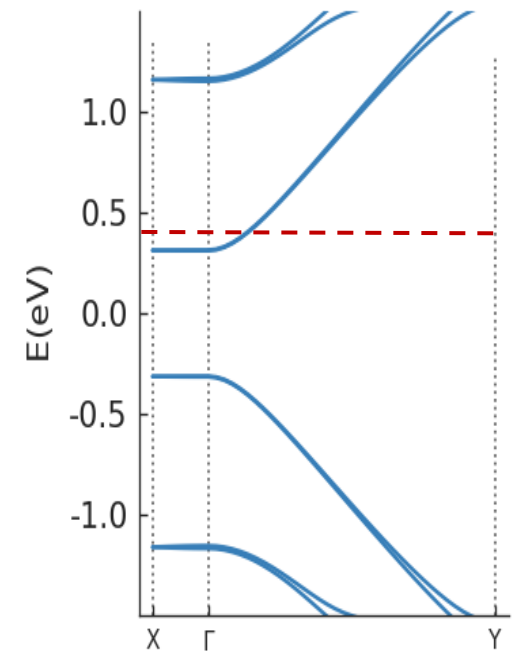
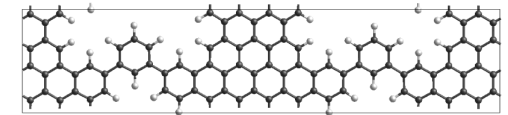
fNPG



para-NPG



meta-NPG



DFT (PBE; Siesta)

LSQT Setup

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Propagation length

$$L_y = \sqrt{\Delta Y^2(E, t)}$$

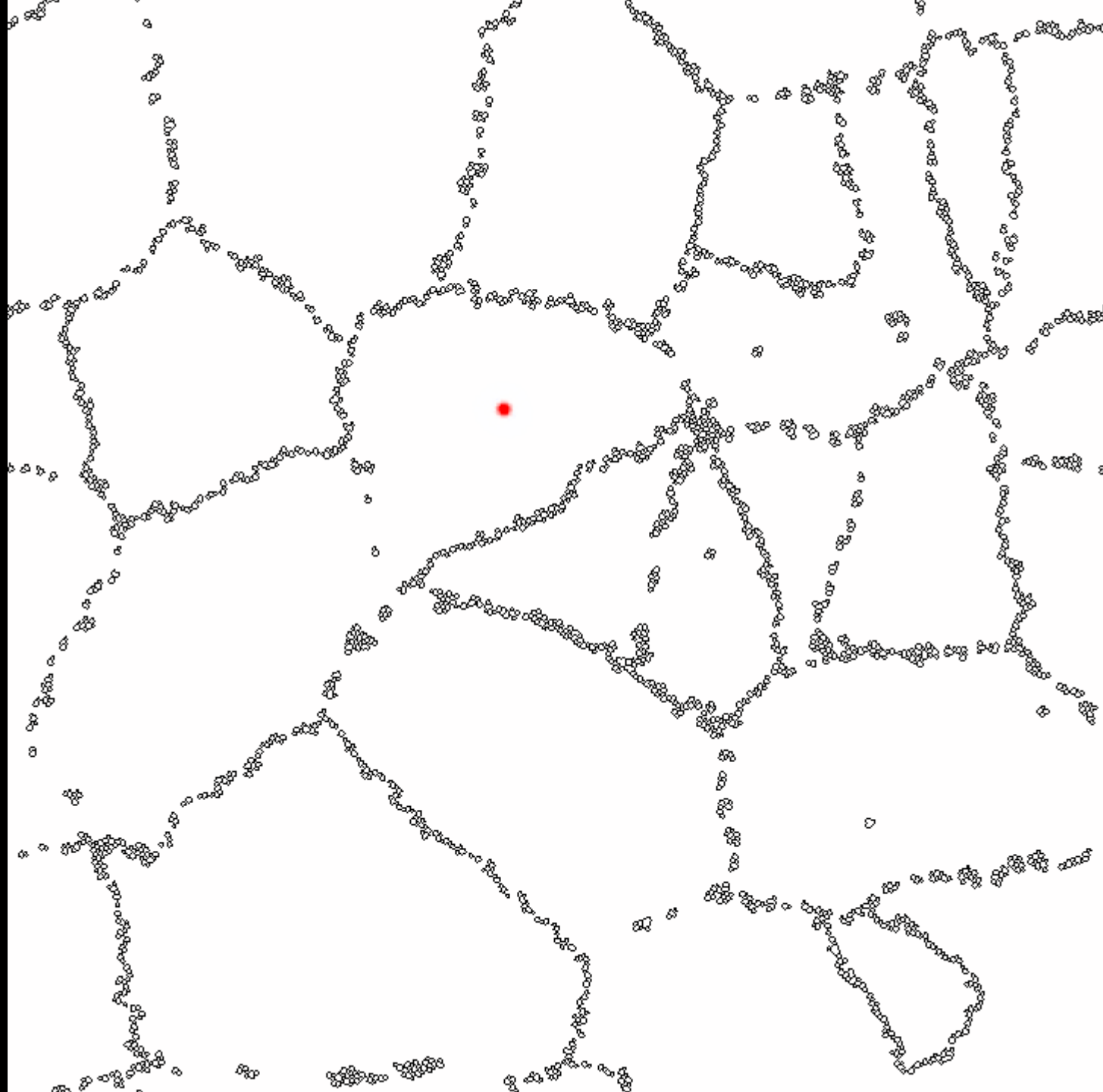
Diffusion coefficient

$$D_y(E, t) = \frac{1}{2} \frac{d\Delta Y^2(E, t)}{dt}$$

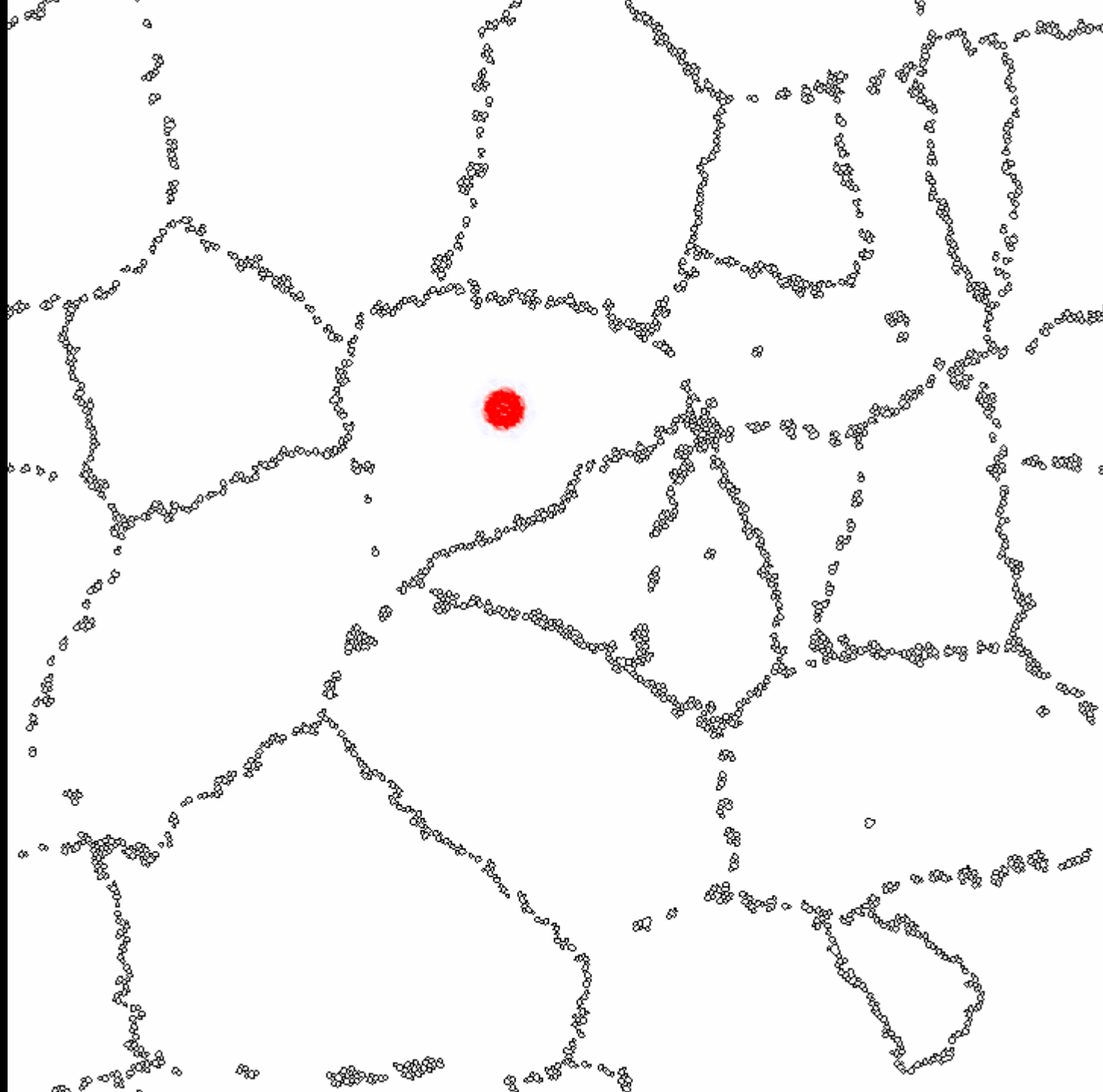
Conductivity

$$\sigma_y(E, t) = D_y(E, t) \cdot \rho(E) \cdot e^2$$

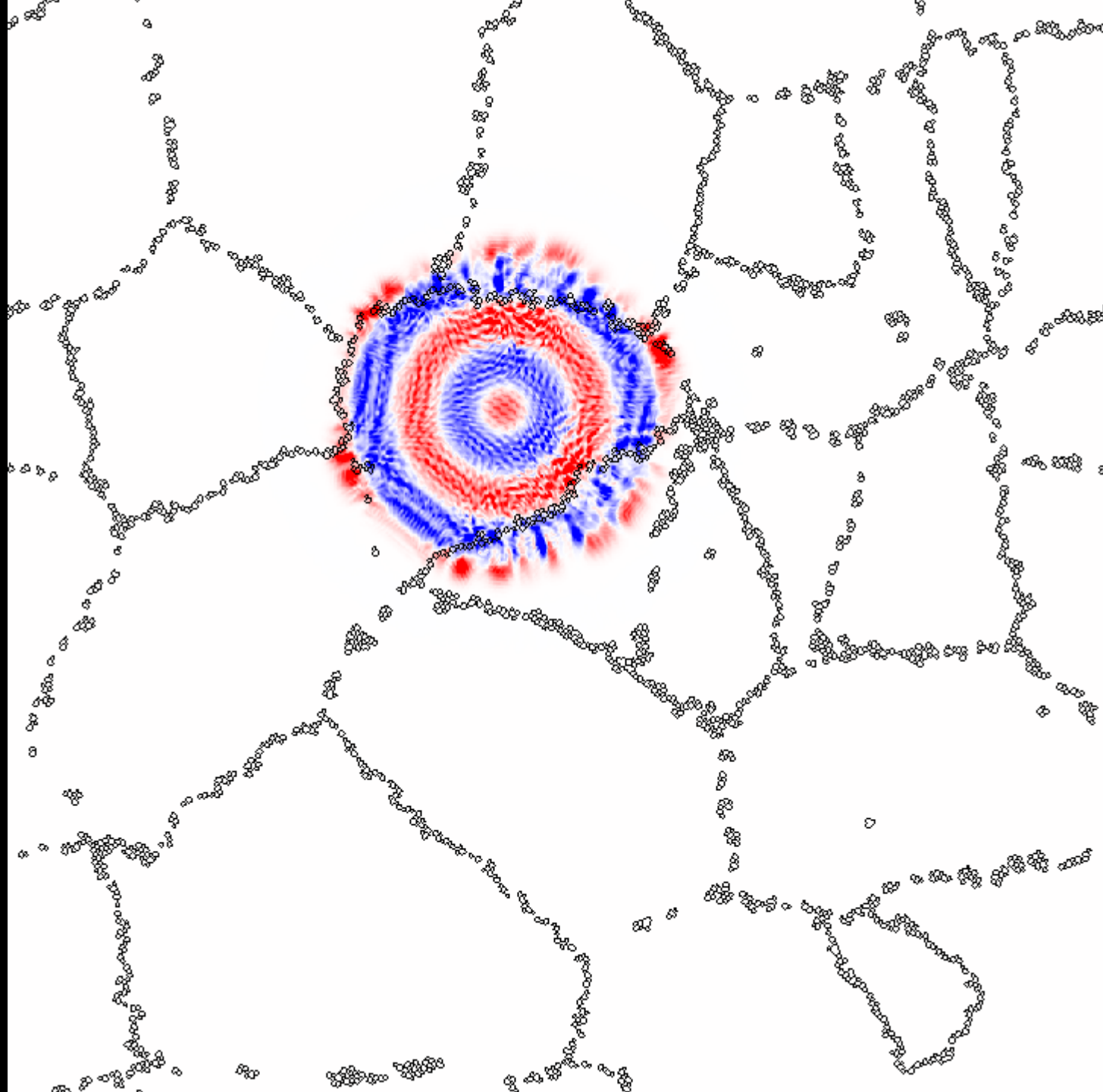
$$A(E) = \sigma_y^{max} / \sigma_x^{max}$$



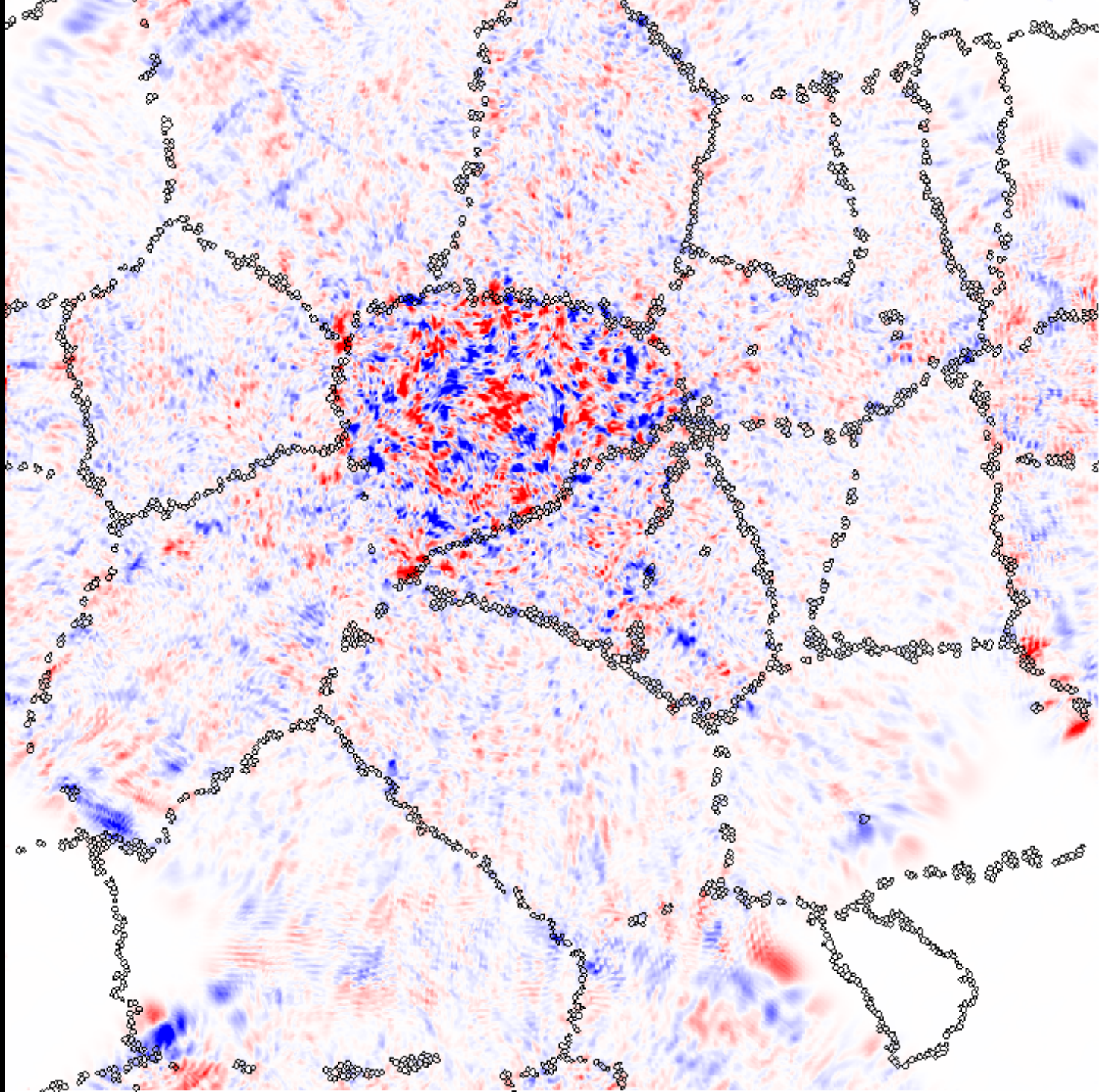
by
A. Cummings



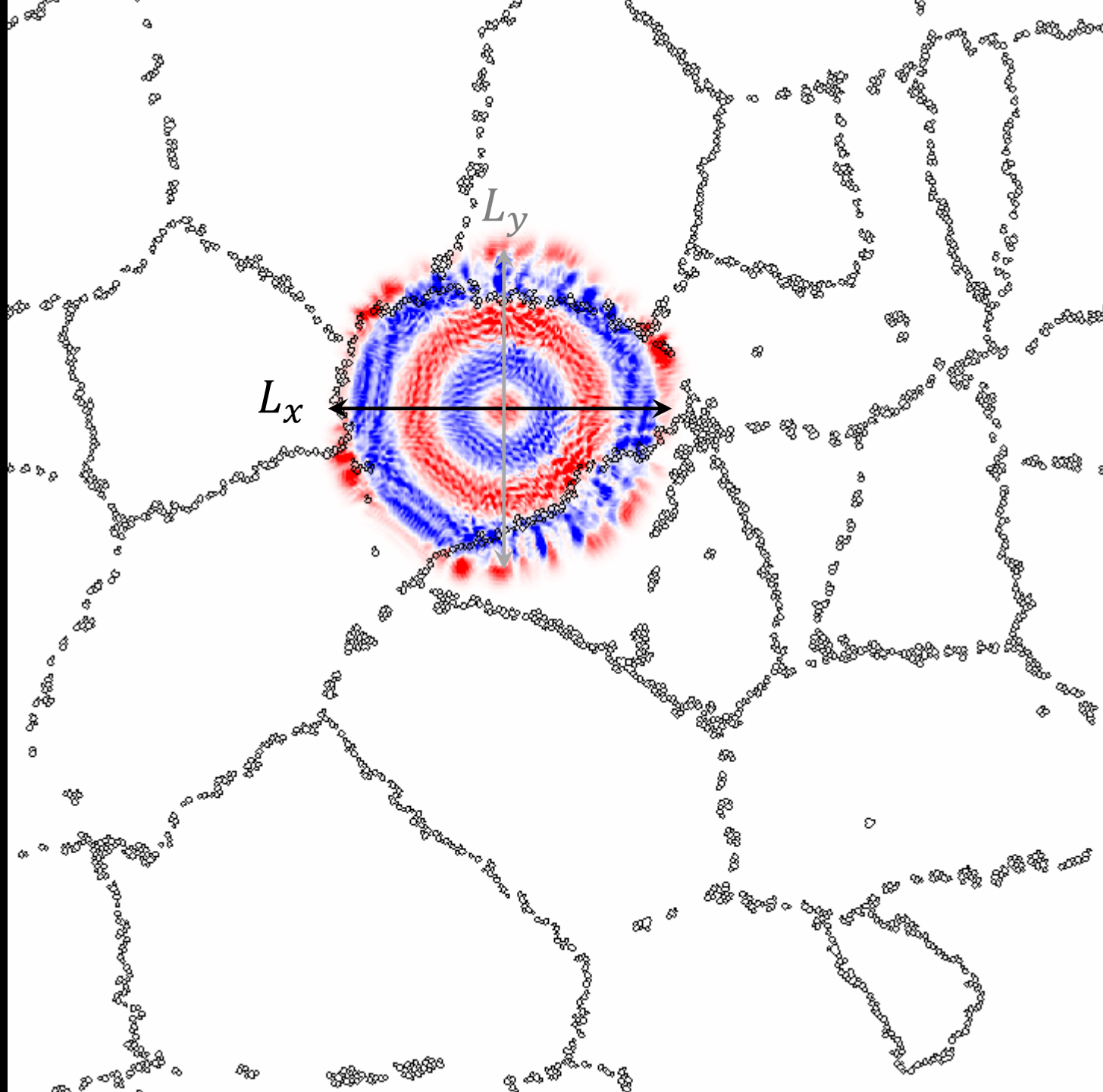
by
A. Cummings



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LSQT Setup

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Conductivity

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Propagation length

$$L_y = \sqrt{\Delta Y^2(E, t)}$$

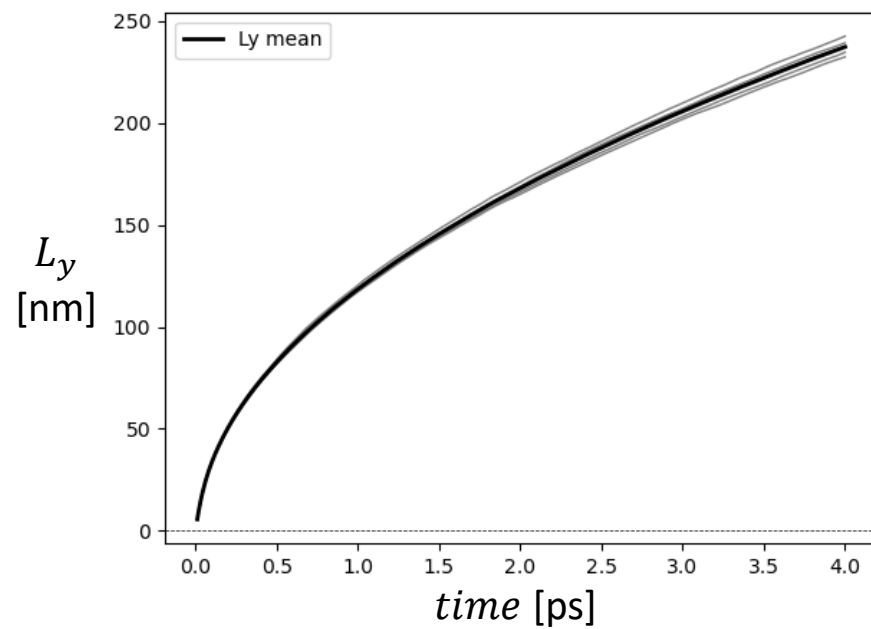
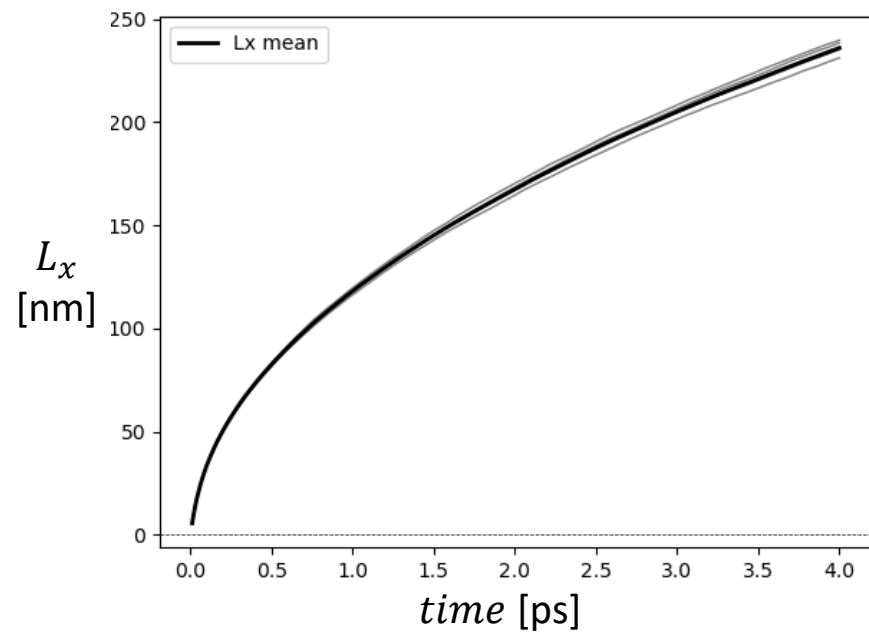
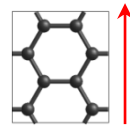
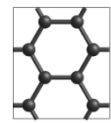
Diffusion coefficient

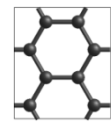
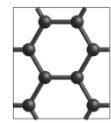
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$$A(E) = \sigma_y^{max} / \sigma_x^{max}$$



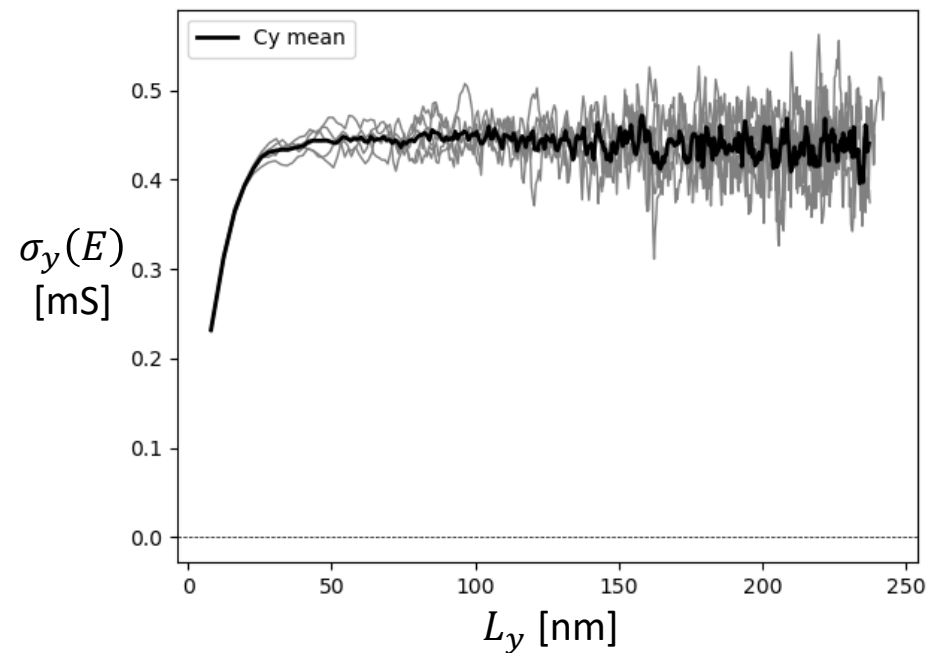
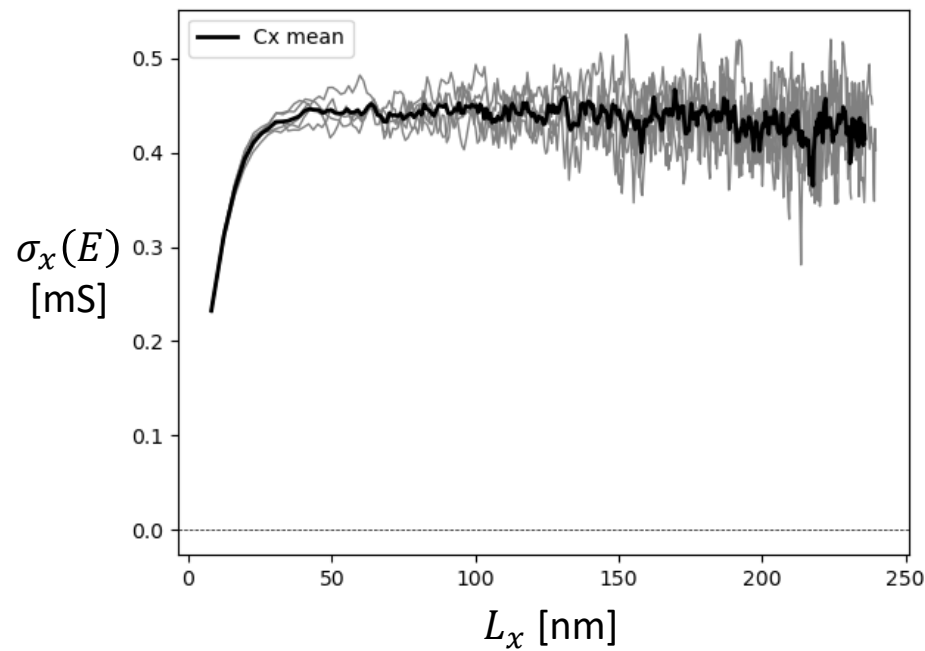


DOS

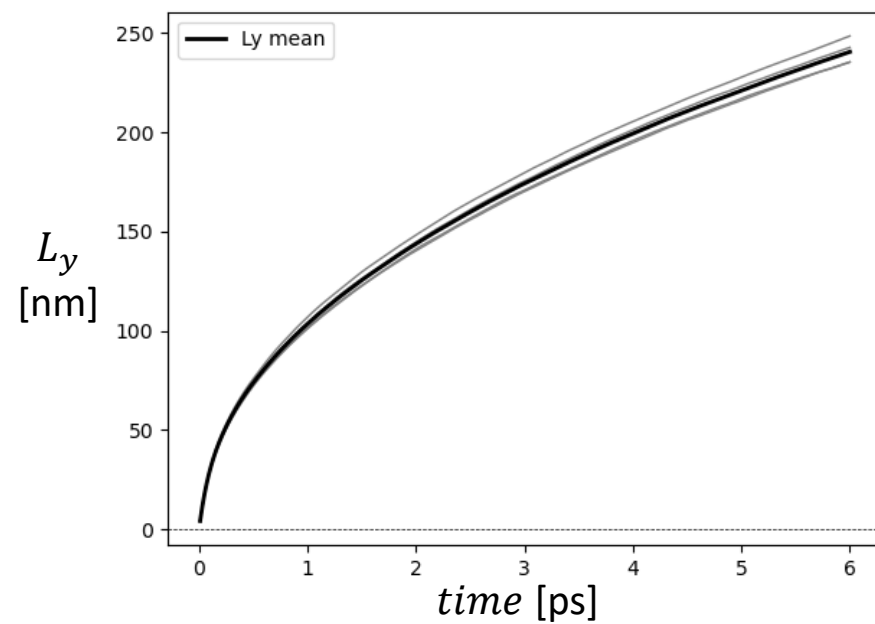
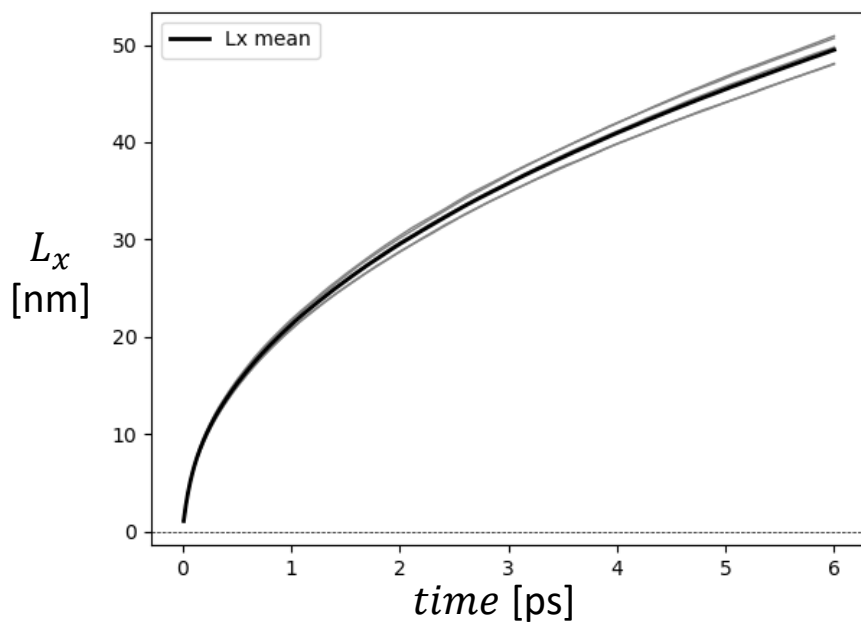
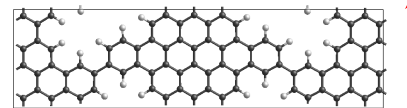
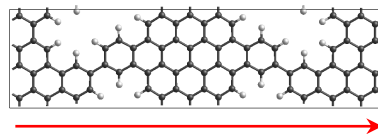
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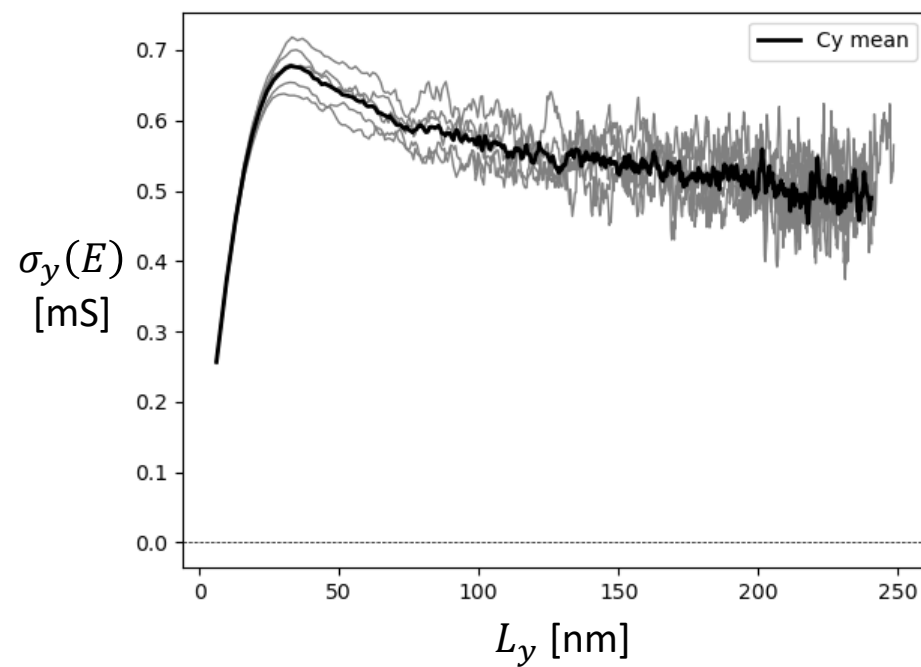
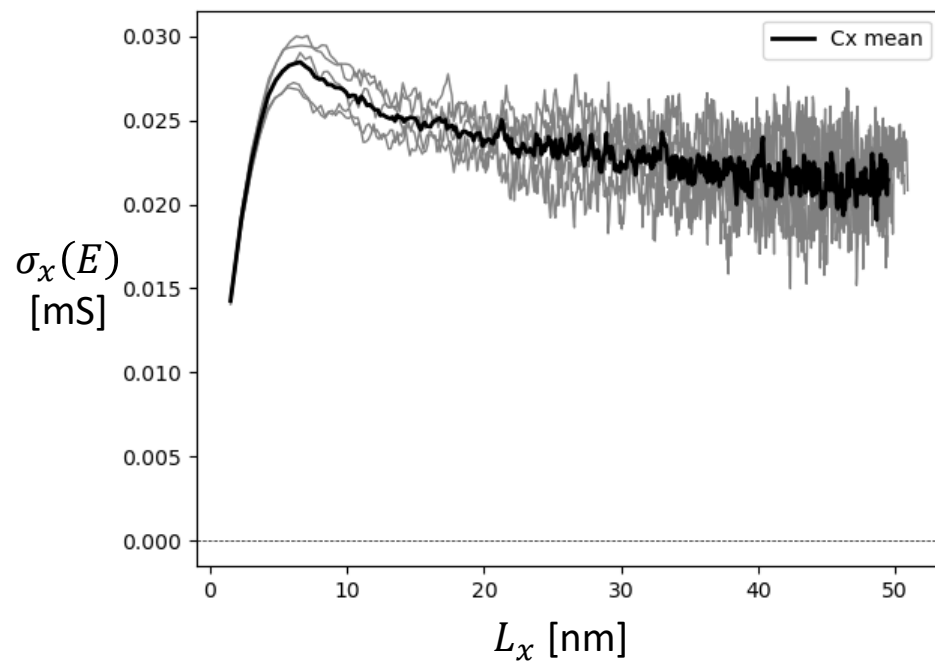
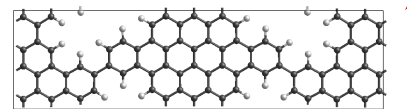
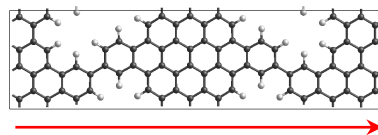
$$\sigma_x(E, t) = D_x(E, t) \cdot \rho(E) \cdot e^2$$

$$\sigma_y(E, t) = D_y(E, t) \cdot \rho(E) \cdot e^2$$



$$A(E) = \sigma_y^{\max} / \sigma_x^{\max} \approx 1$$





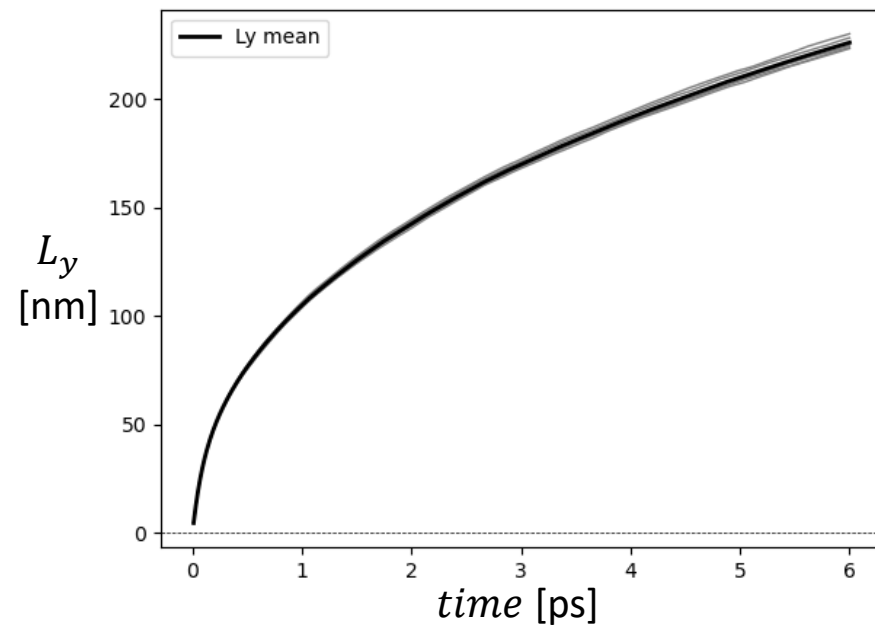
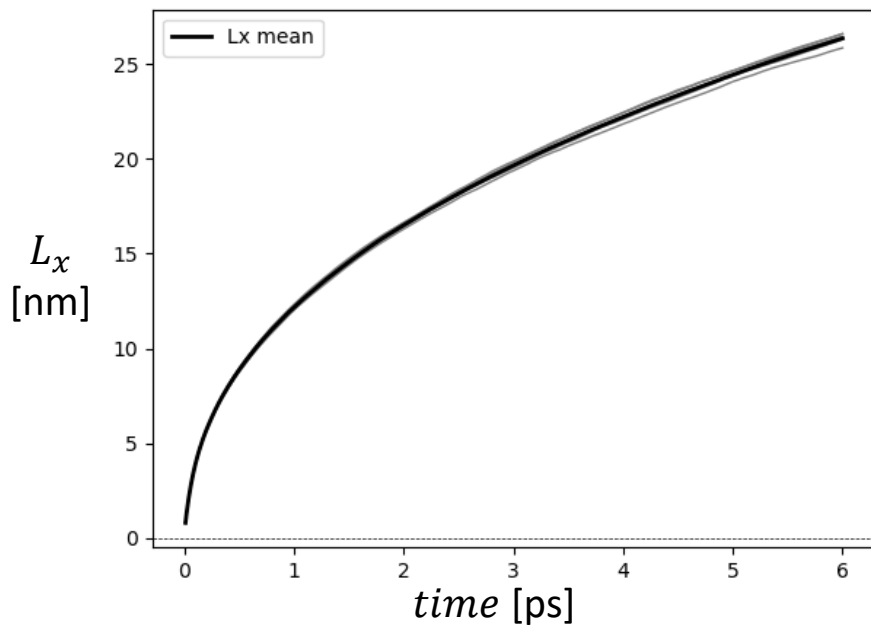
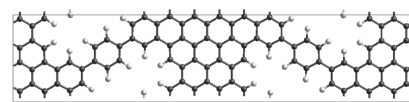
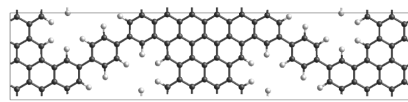
$$A(E) = \sigma_y^{\max} / \sigma_x^{\max} \approx 25$$

paraNPG

X

Y

$$E_F = 0.4 \text{ eV}$$

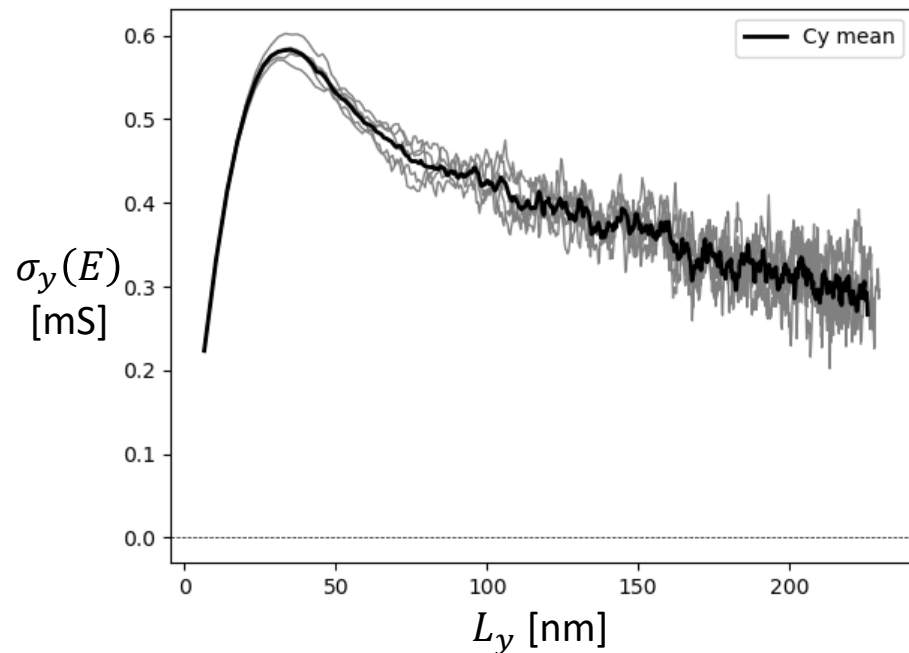
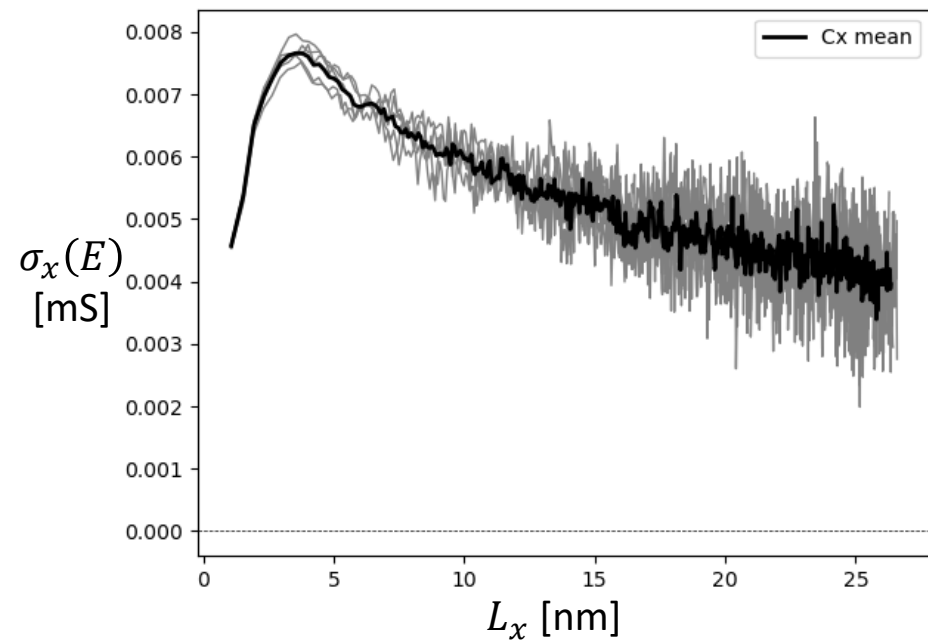
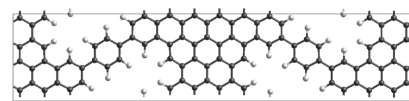
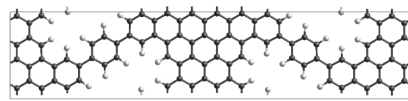


paraNPG

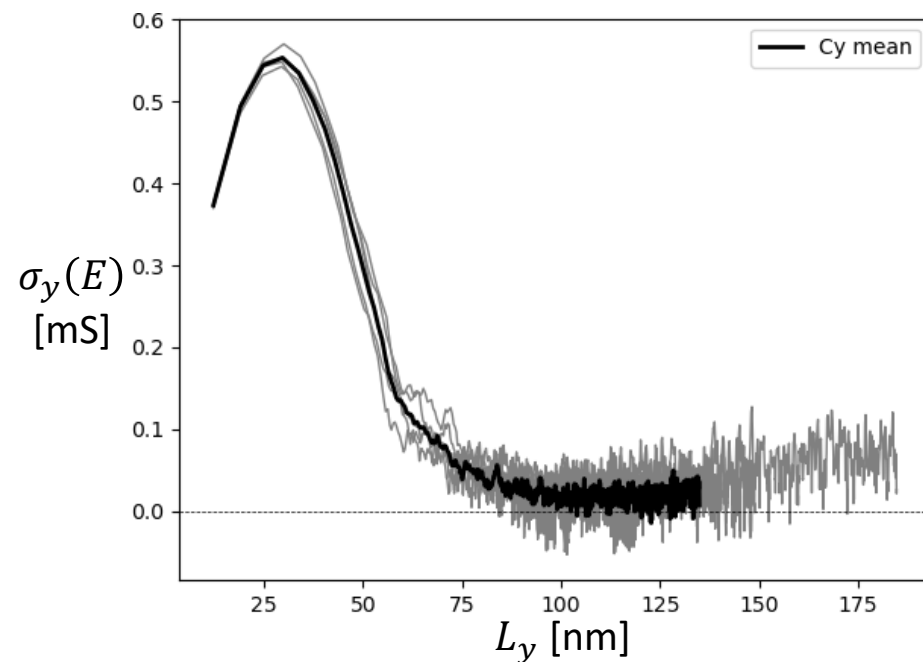
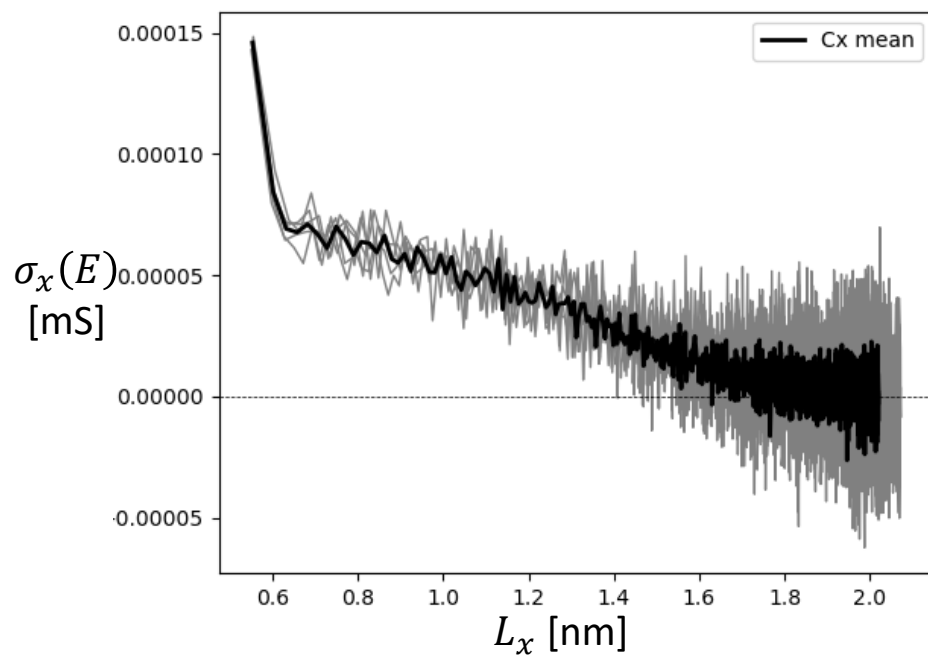
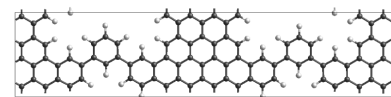
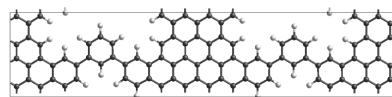
X

Y

$$E_F = 0.4 \text{ eV}$$



$$A(E) = \sigma_y^{\max} / \sigma_x^{\max} \approx 80$$



$$A(E) = \sigma_y^{\max} / \sigma_x^{\max} \approx \infty$$

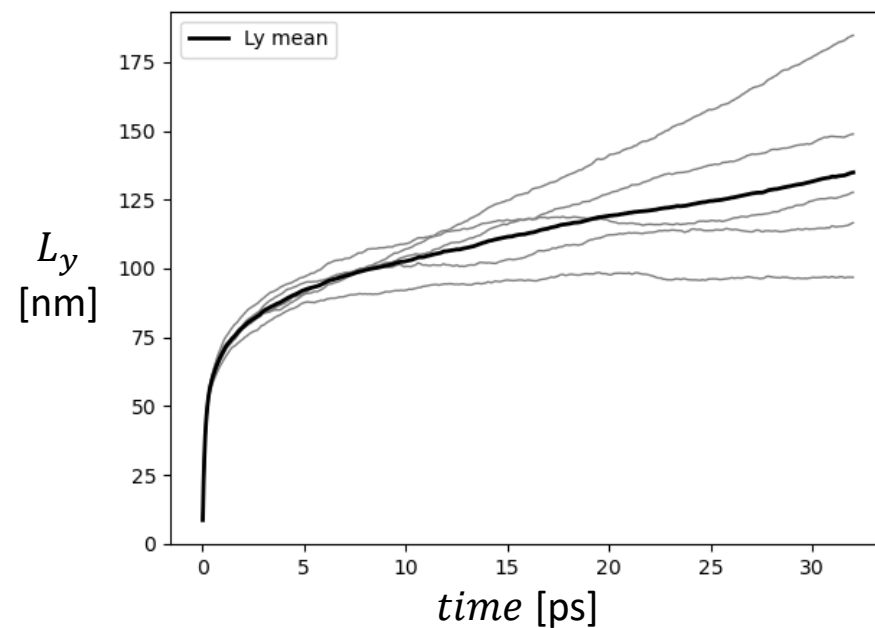
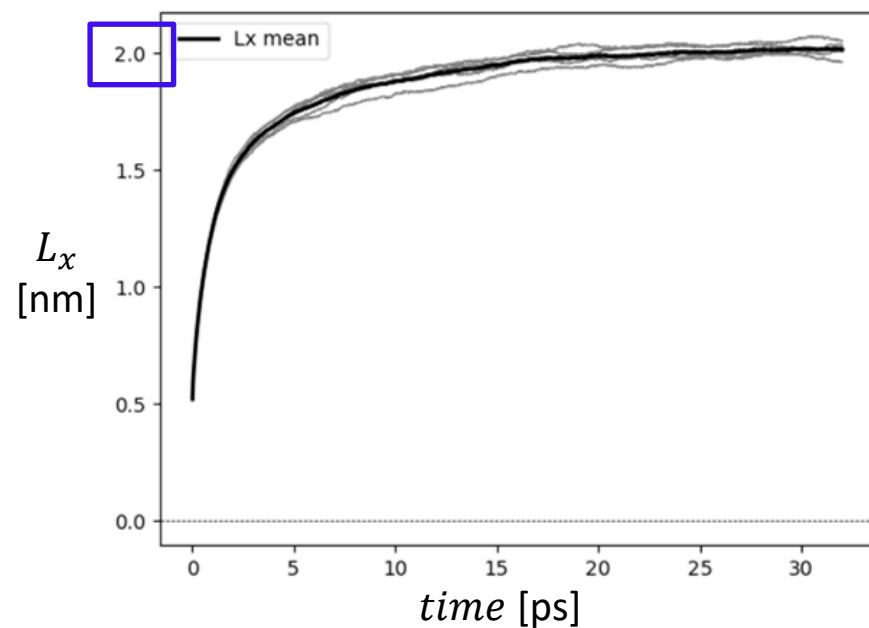
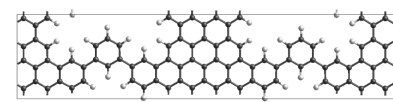
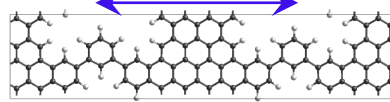
metaNPG

X

Y

$$E_F = 0.4 \text{ eV}$$

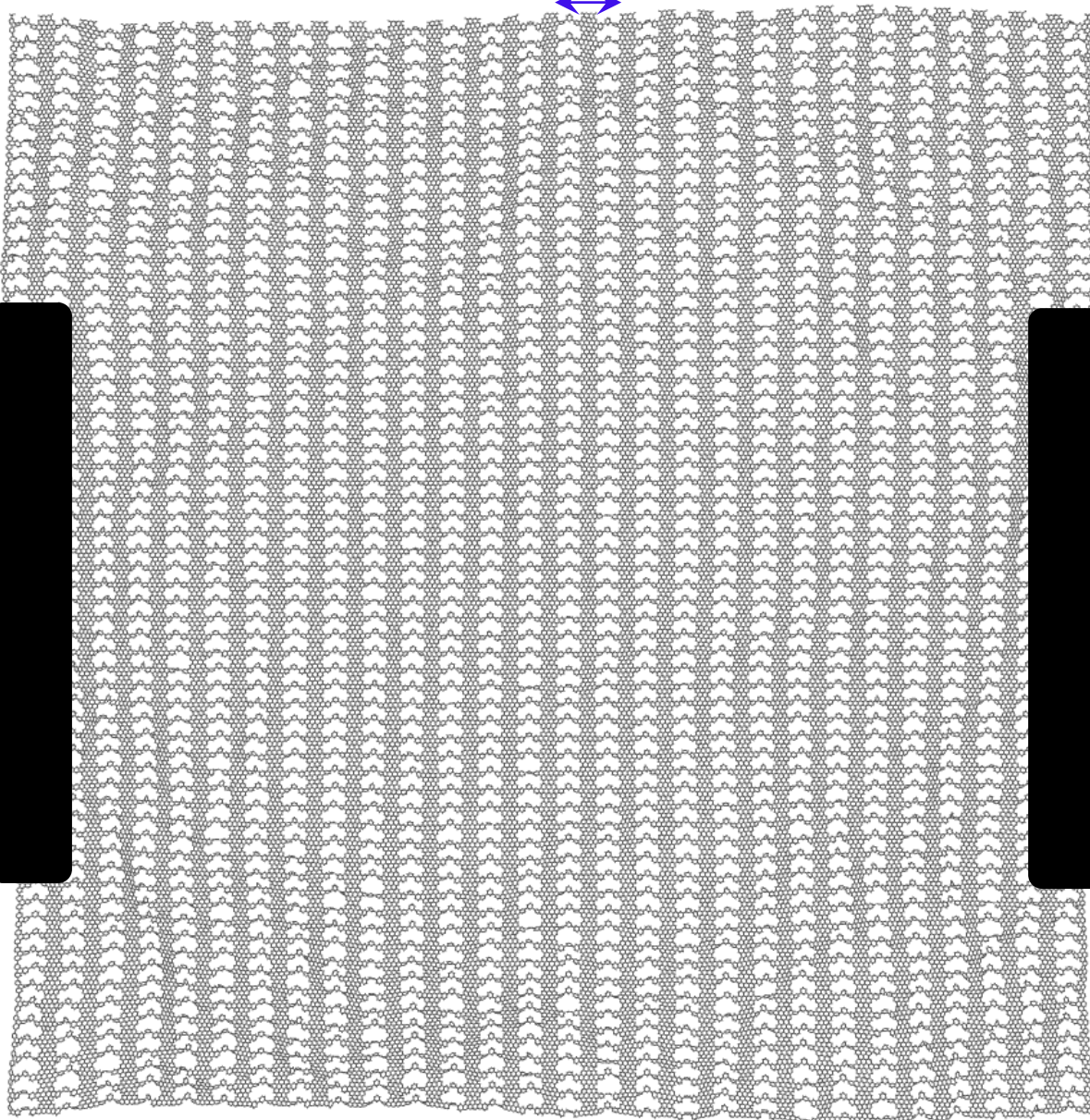
2 nm



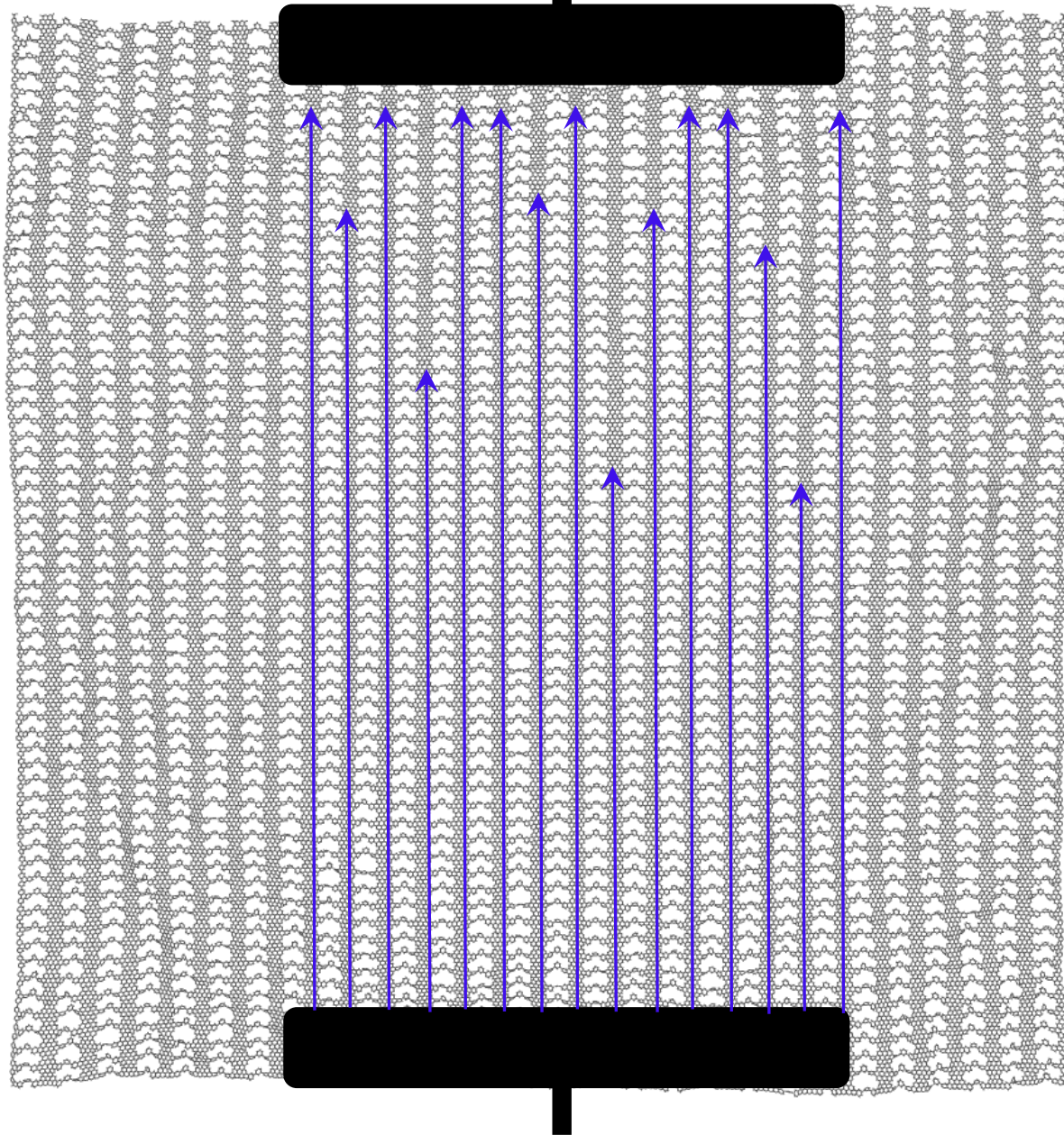
$$A(E) \approx \infty$$

metaNPG

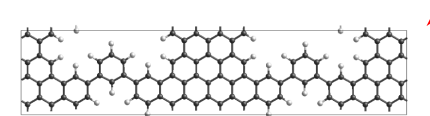
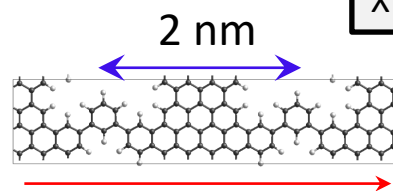
2 nm



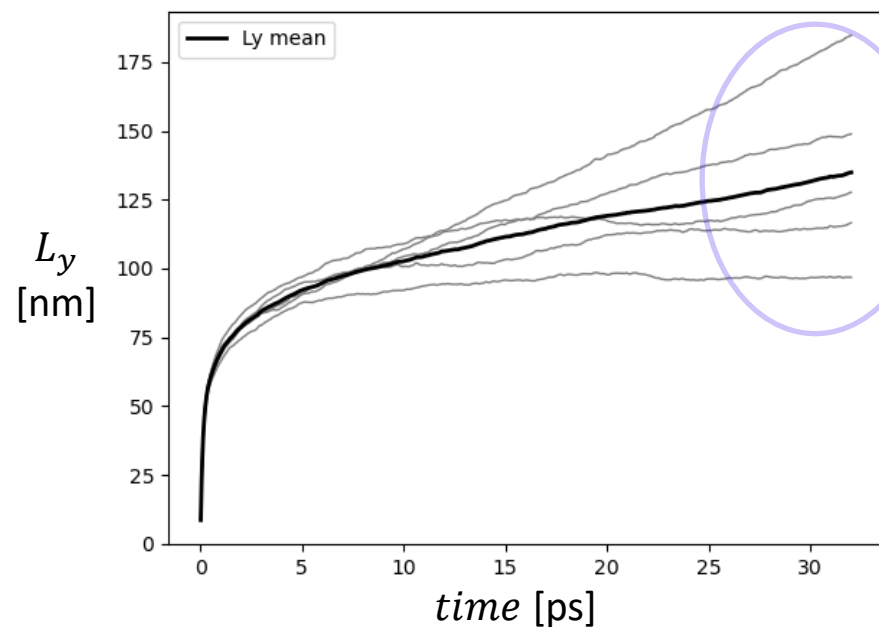
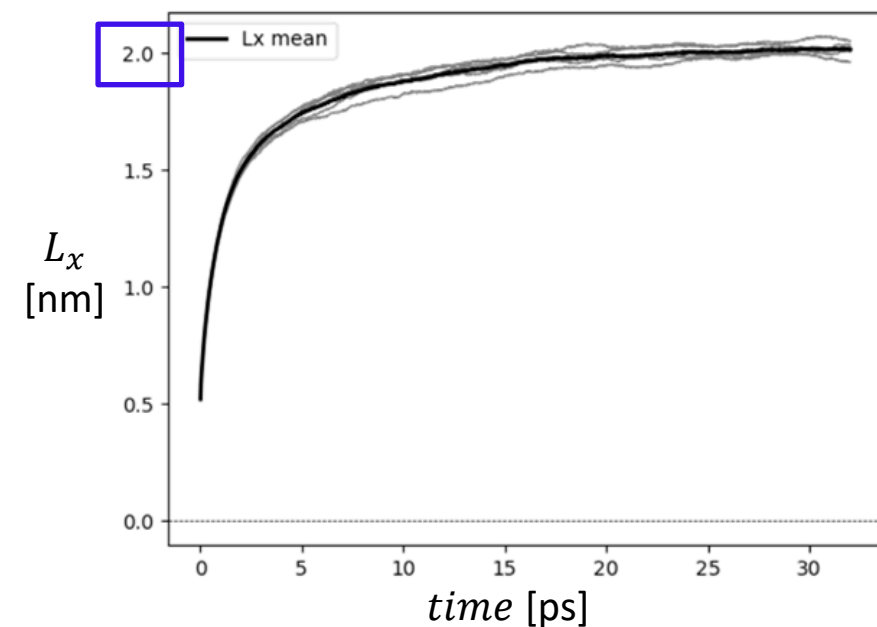
$$A(E) \approx \infty$$



$$A(E) \approx \infty$$



atomic/molecular sensing



$$A(E) \approx \infty$$

Pristine ✓

Disordered ✓

Concluding...

2D materials

atomic/molecular sensing

Graphene



fabNPG



paraNPG



metaNPG

$$A(E) \approx 1$$

$$A(E) \approx 25$$

$$A(E) \approx 80$$

$$A(E) \approx \infty$$

2D charge transport

1D charge transport



Thanks for listening



MINISTERIO
DE CIENCIA, INNOVACIÓN
Y UNIVERSIDADES

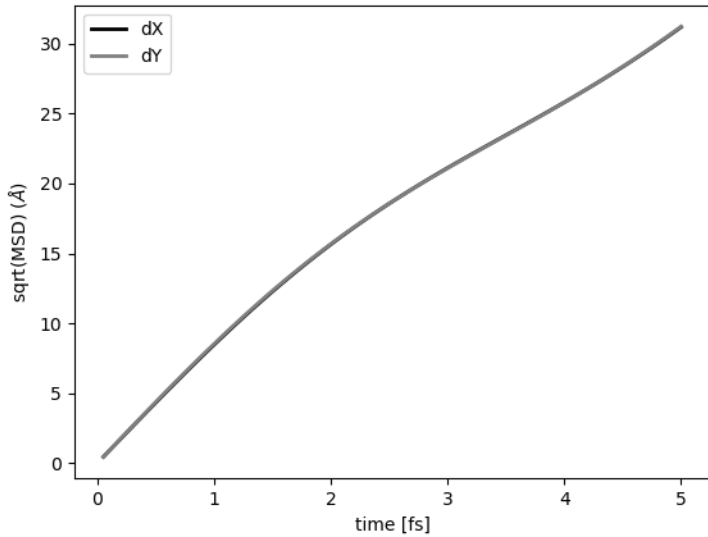


JUAN DE LA CIERVA-FORMACIÓN
FJC2019-038971-I

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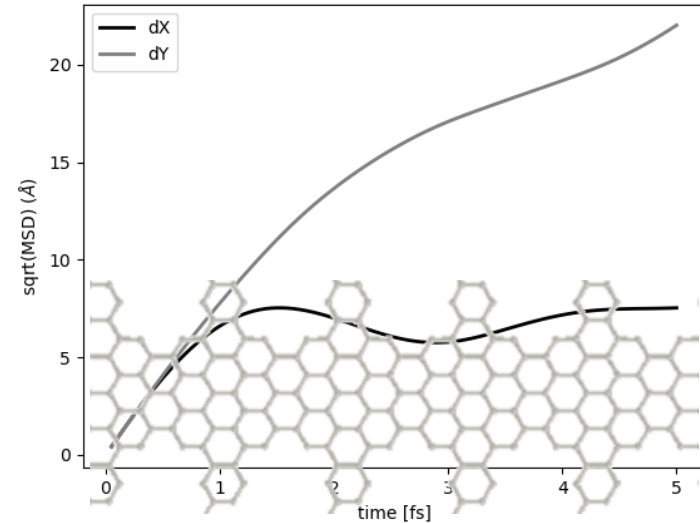
Pristine systems – Ballistic regime (LSQT)

$E - E_F = 0.40000000000000013$ eV



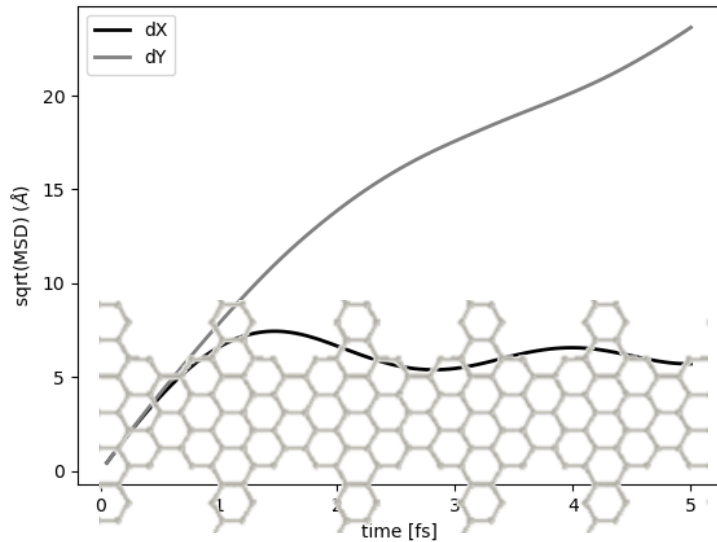
Gr

$E - E_F = 0.40000000000000013$ eV



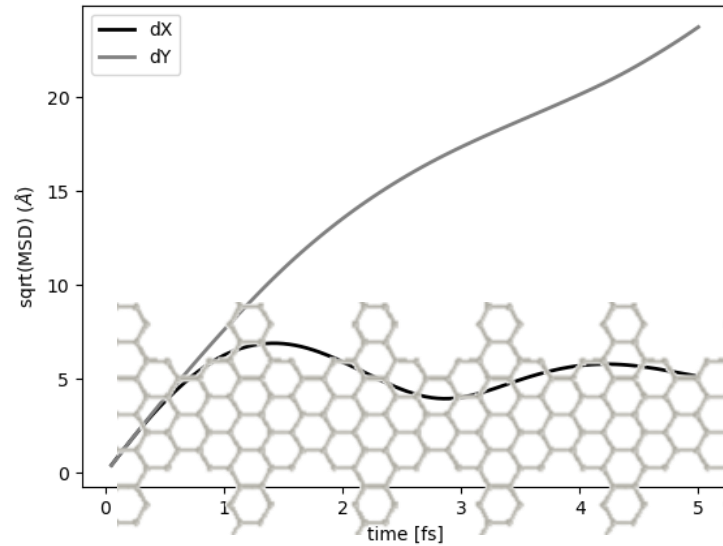
fNPG

$E - E_F = 0.40000000000000013$ eV



pNPG

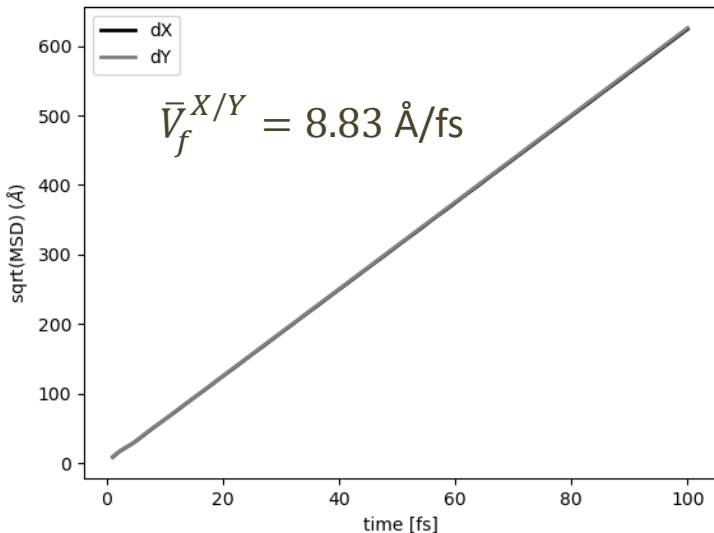
$E - E_F = 0.40000000000000013$ eV



mNPG

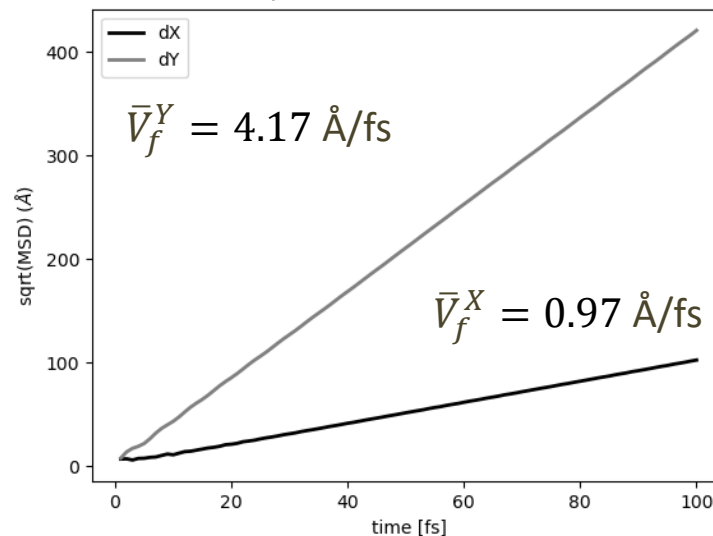
Pristine systems – Ballistic regime (LSQT)

$E - E_F = 0.4$ eV



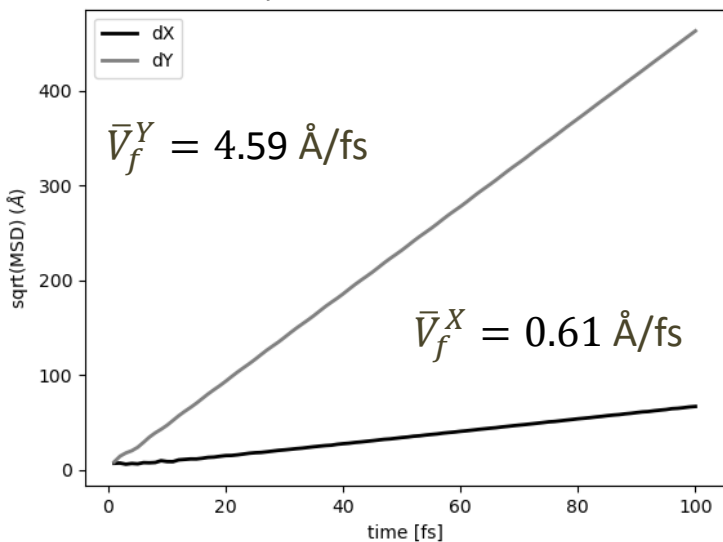
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$E - E_F = 0.400000000000000013$ eV



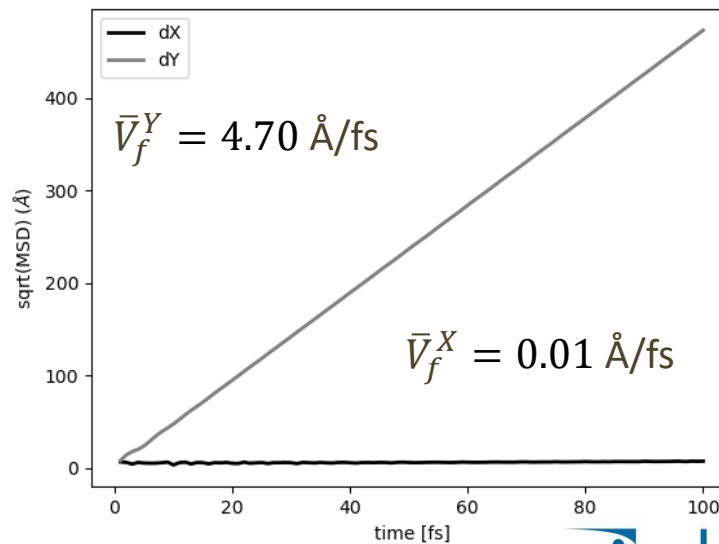
fNPG

$E - E_F = 0.400000000000000013$ eV



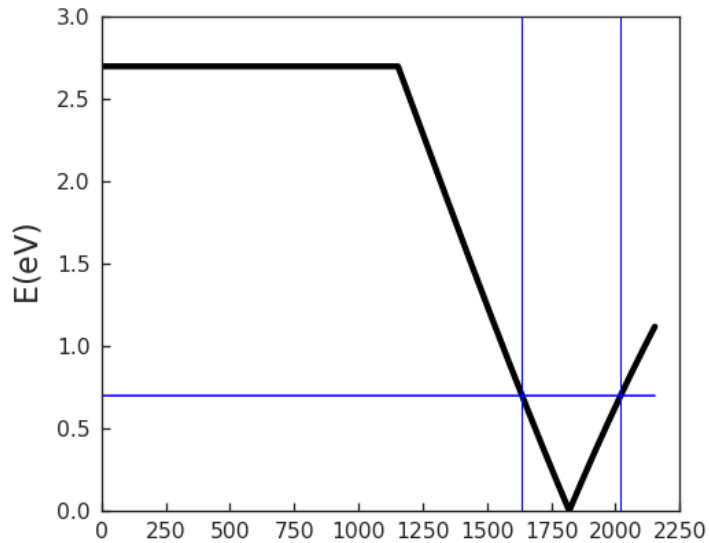
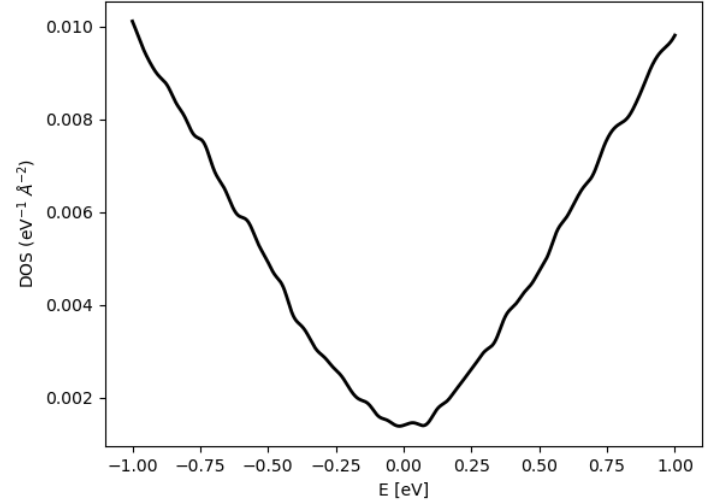
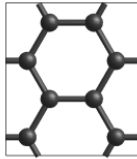
pNPG

$E - E_F = 0.400000000000000013$ eV



mNPG

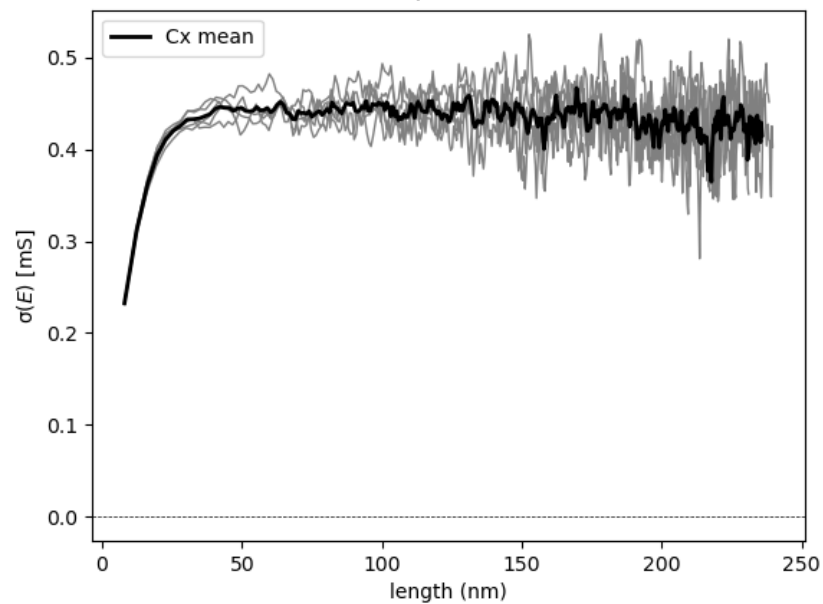
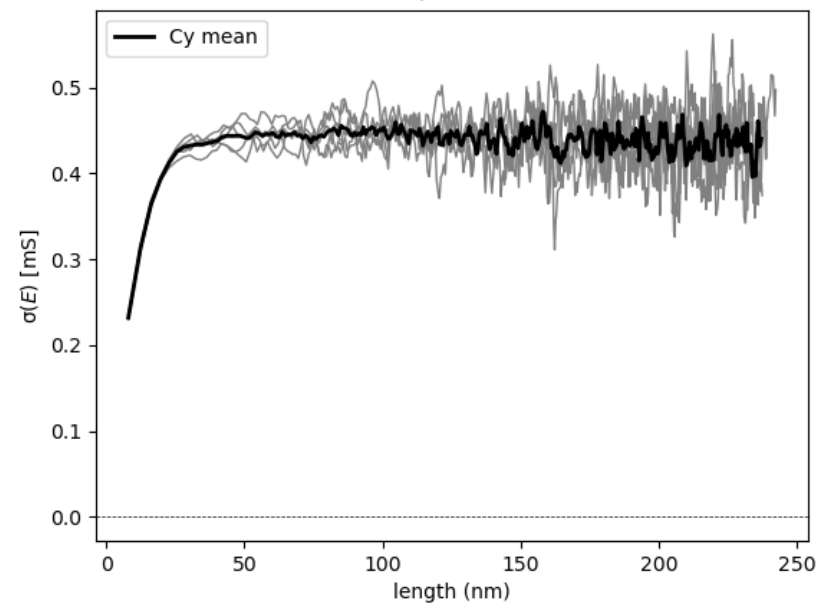
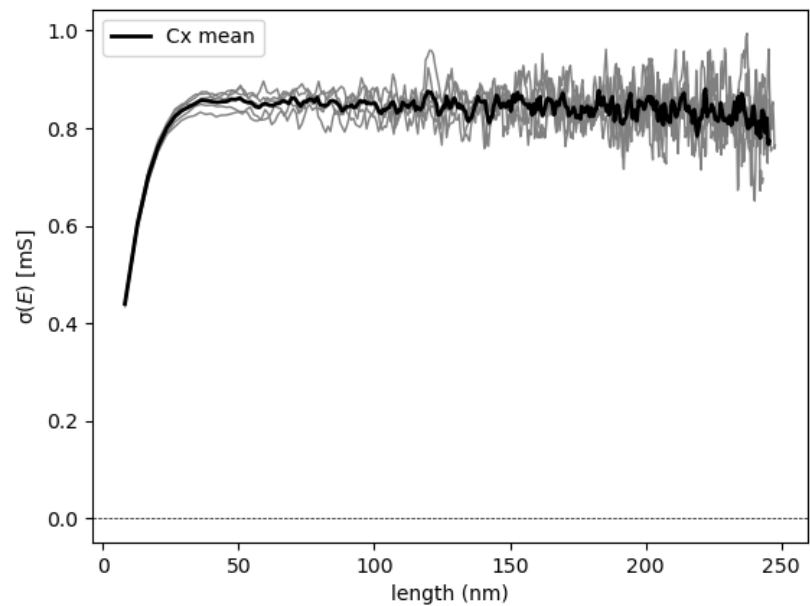
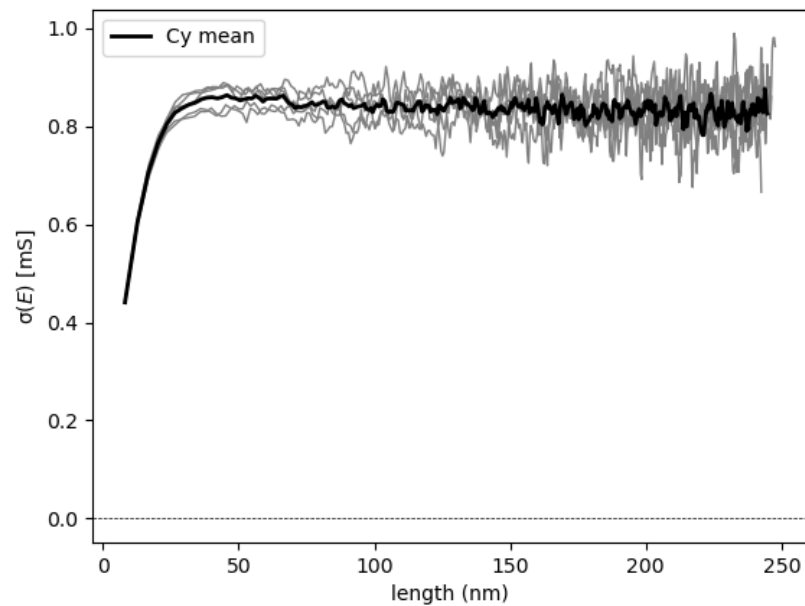
LSQT results: Graphene



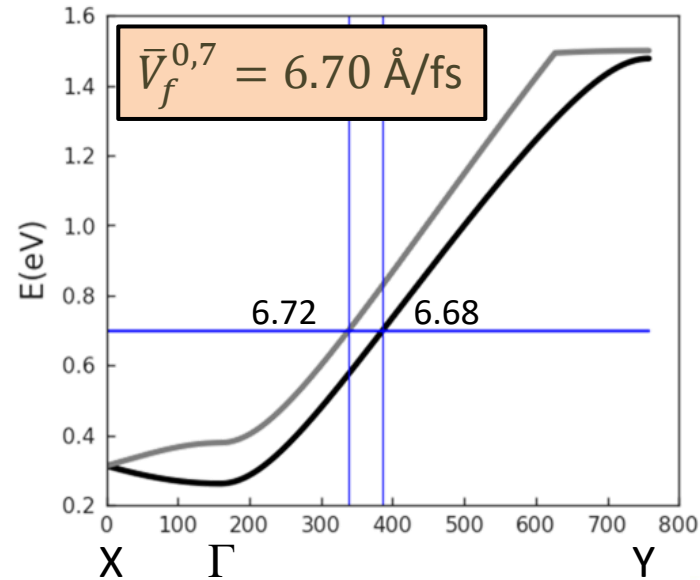
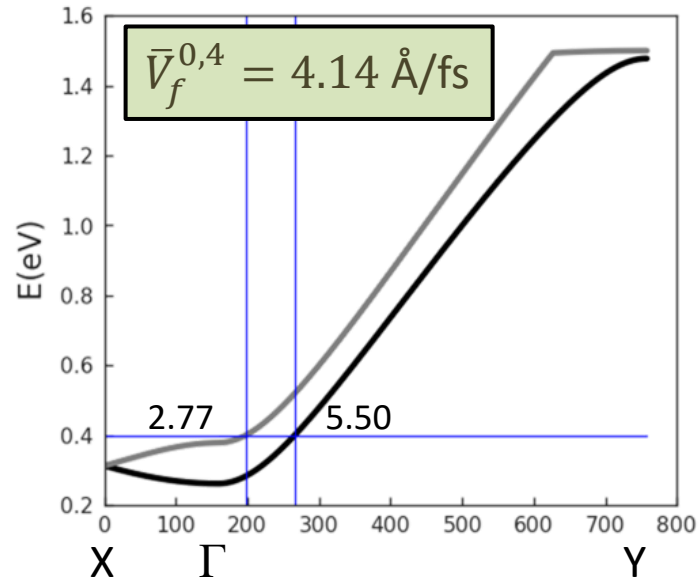
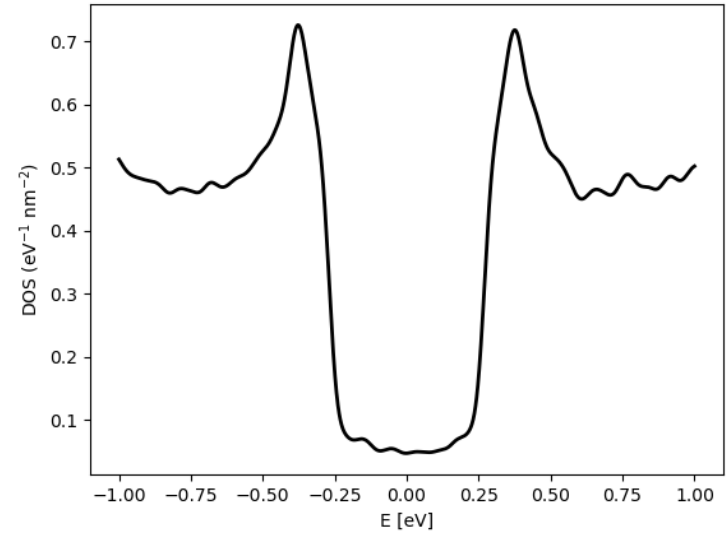
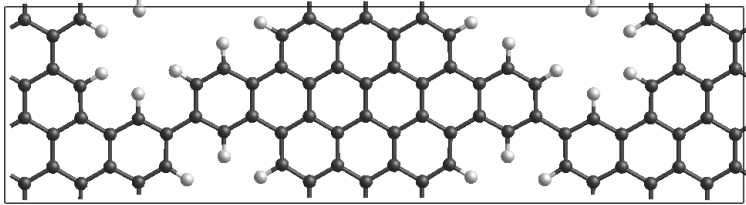
$$\bar{V}_f^{0,4} = 8.83 \text{ \AA/fs}$$

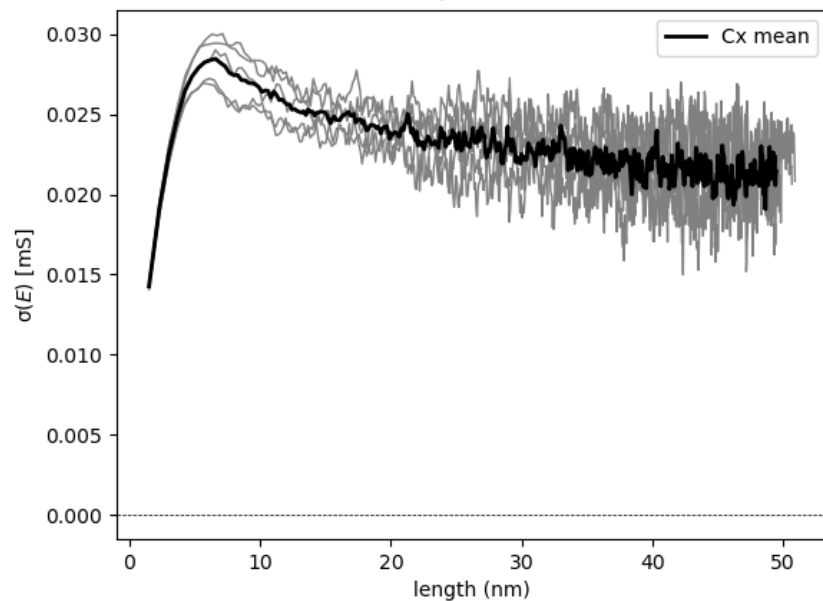
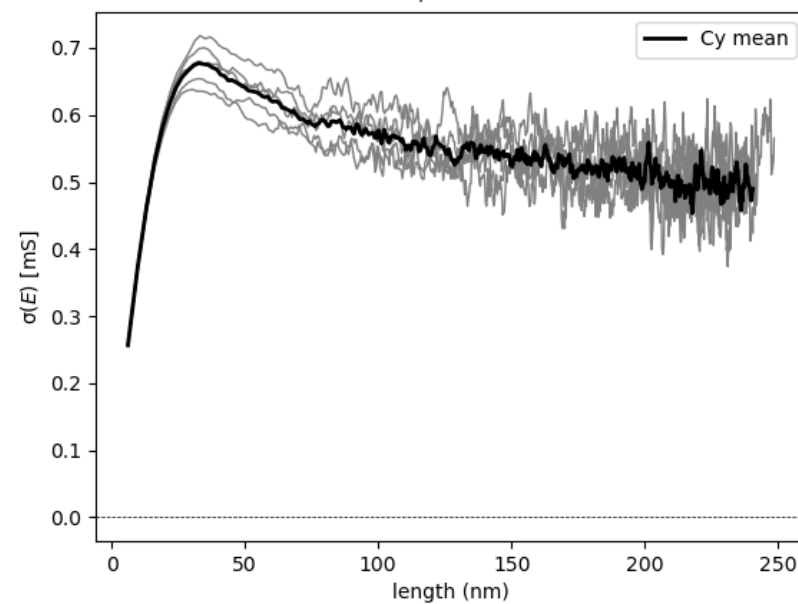
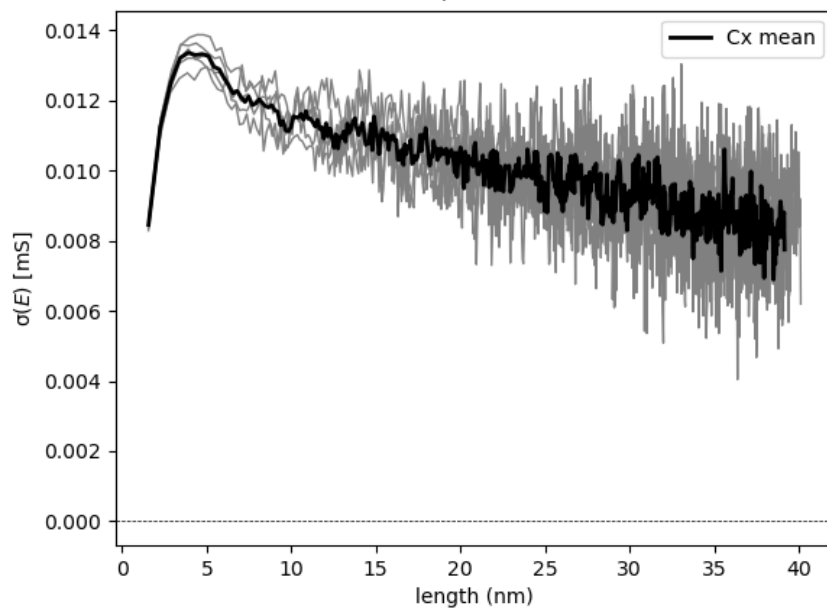
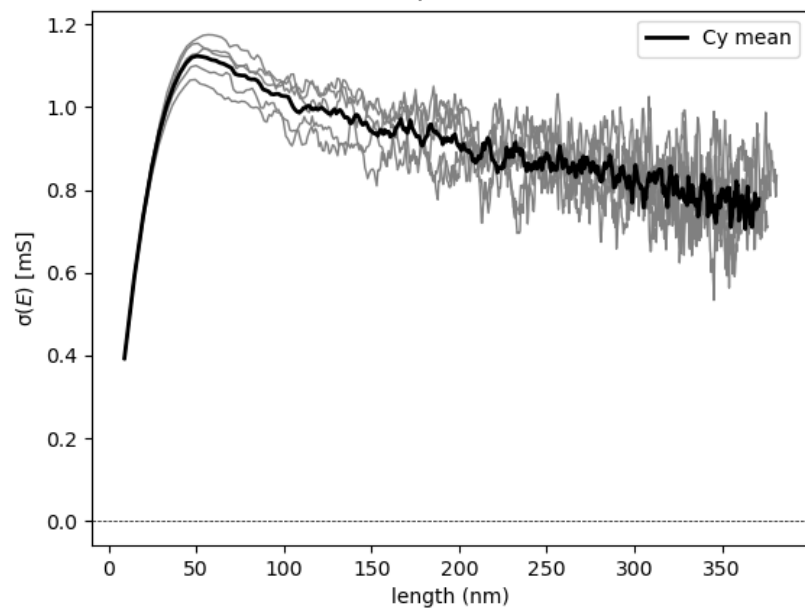
$$\bar{V}_f^{0,7} = 8.74 \text{ \AA/fs}$$

Graphene

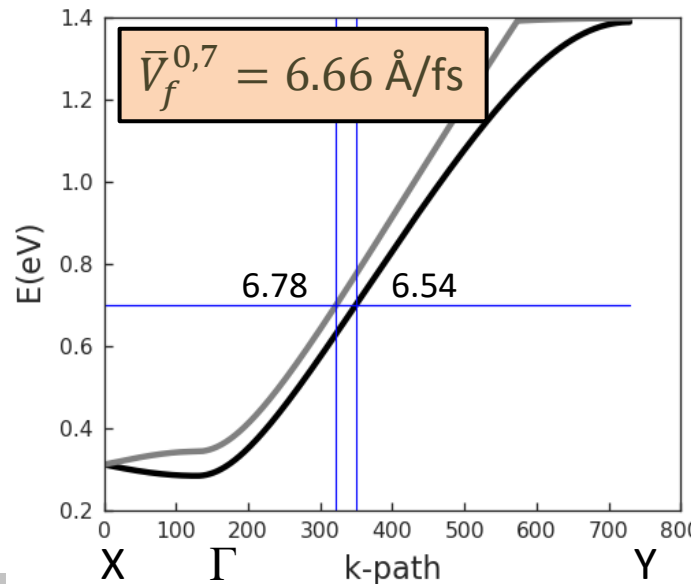
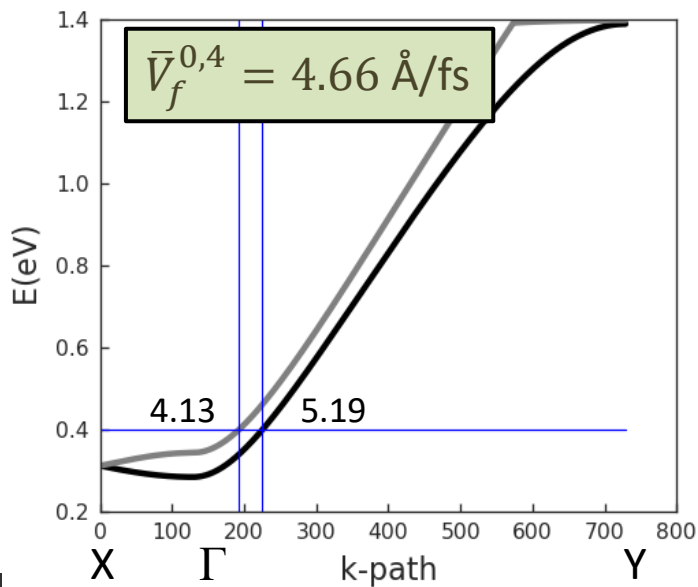
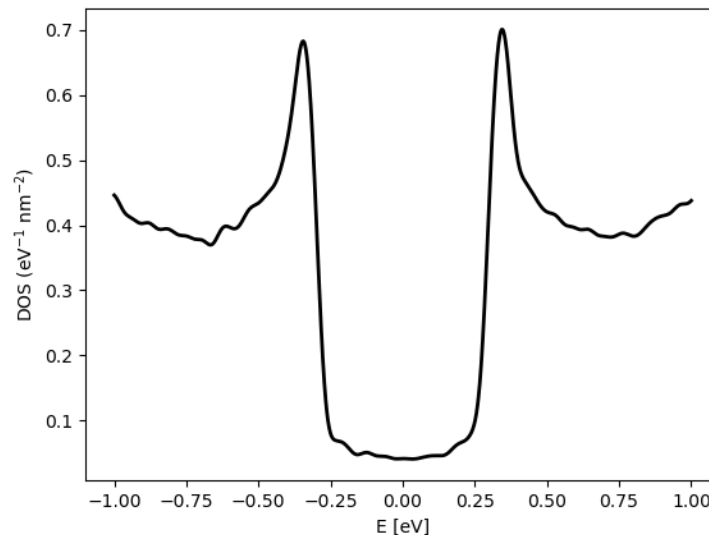
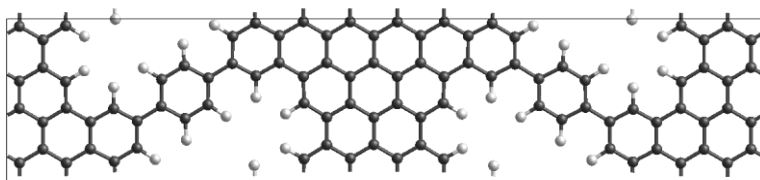
X**Y** $E - E_F = 0.4 \text{ eV}$  $E - E_F = 0.4 \text{ eV}$  $E - E_F = 0.7 \text{ eV}$  $E - E_F = 0.7 \text{ eV}$ 

LSQT results: fab-NPG



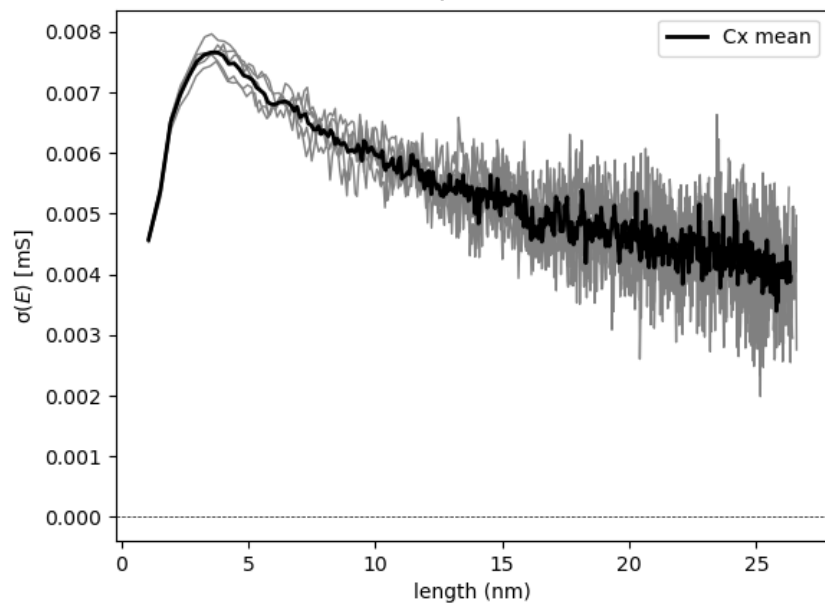
$E - E_F = 0.4$ eV $E - E_F = 0.4$ eV $E - E_F = 0.7$ eV $E - E_F = 0.7$ eV

LSQT results: para-NPG



paraNPG

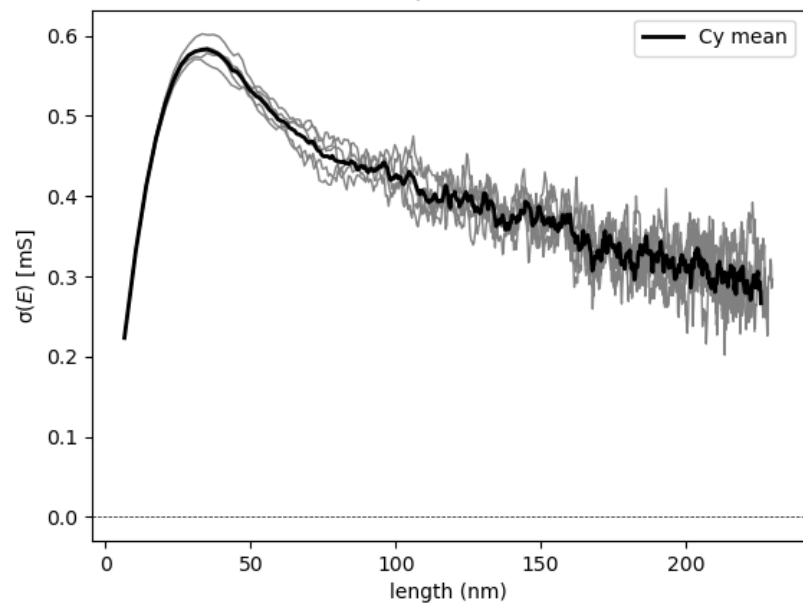
$E - E_F = 0.4$ eV



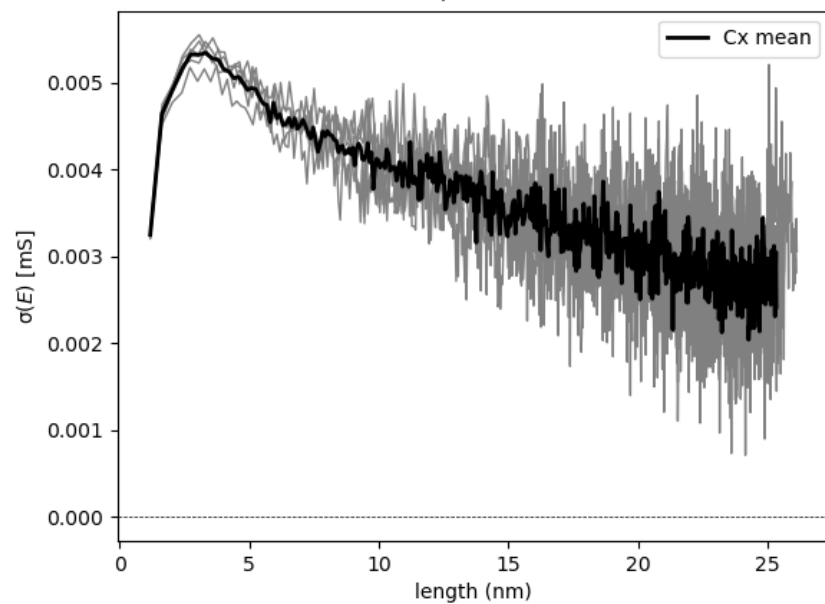
X

Y

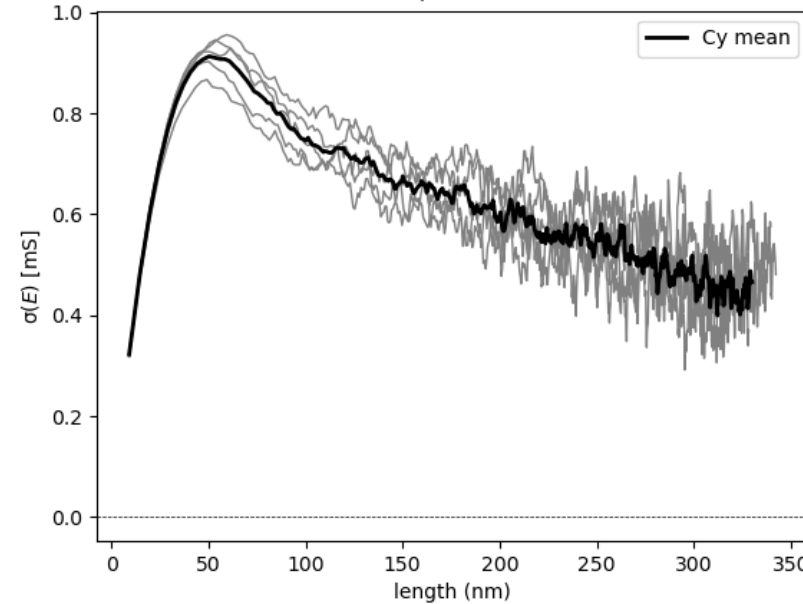
$E - E_F = 0.4$ eV



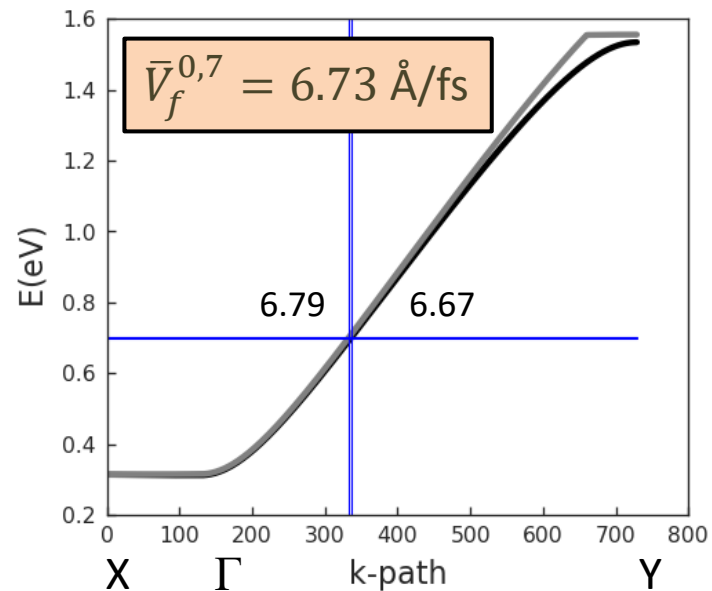
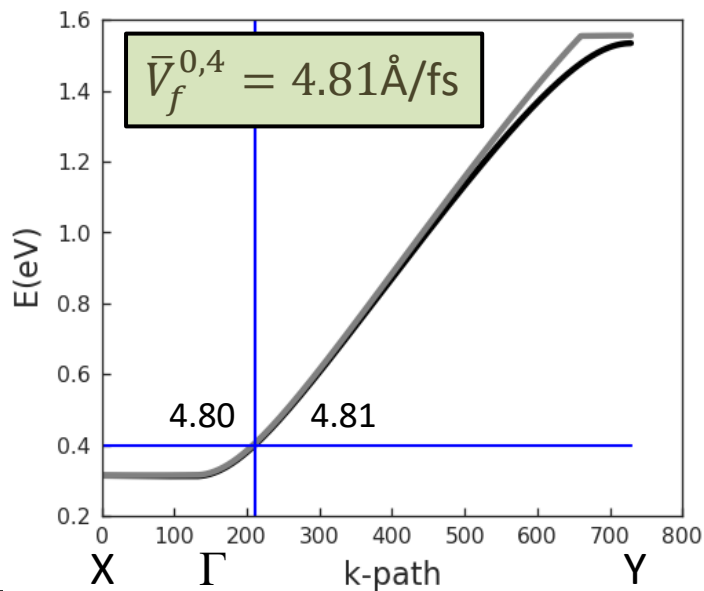
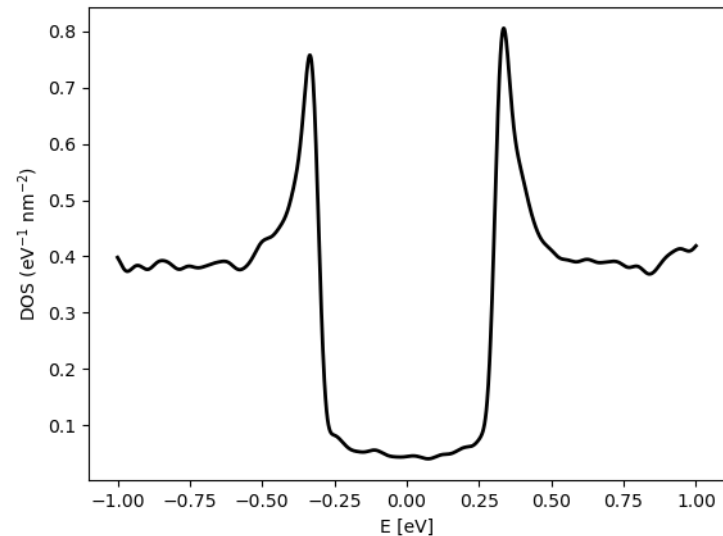
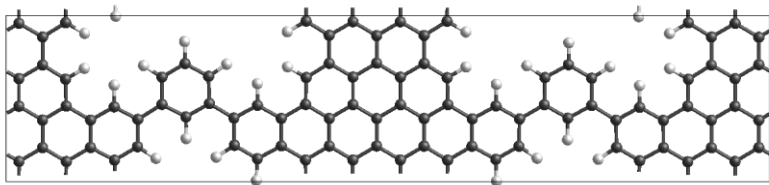
$E - E_F = 0.7$ eV



$E - E_F = 0.7$ eV



LSQT results: meta-NPG



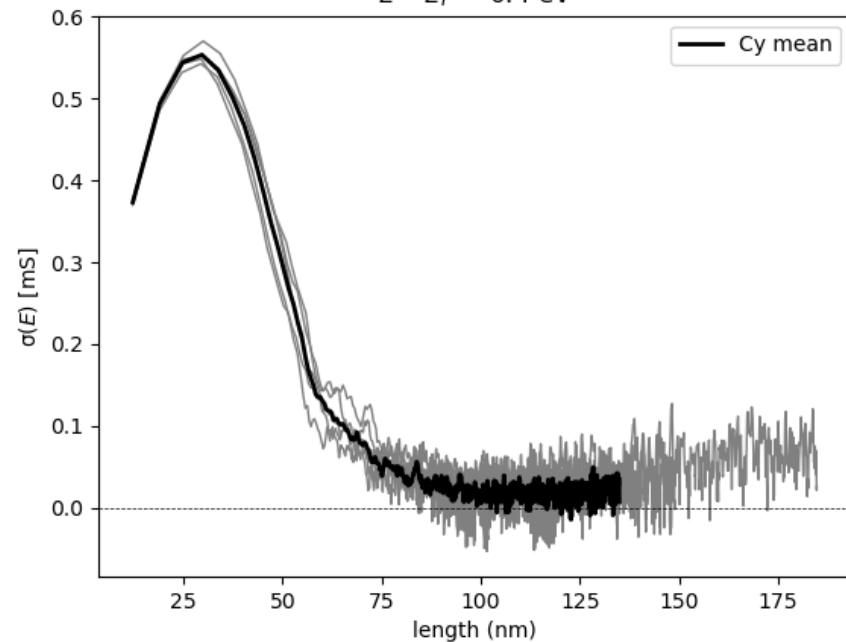
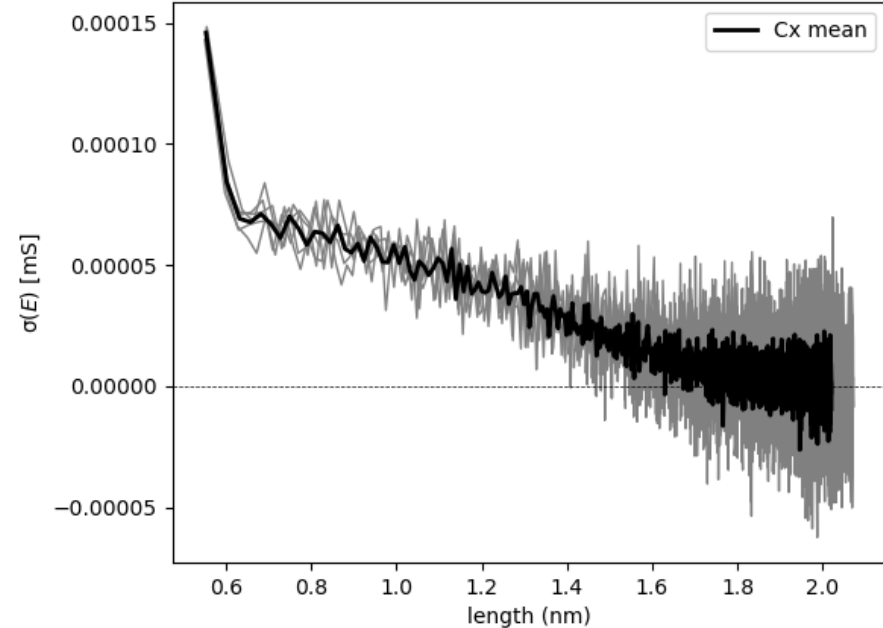
metaNPG

X

Y

$E - E_F = 0.4$ eV

$E - E_F = 0.4$ eV



$E - E_F = 0.7$ eV

$E - E_F = 0.7$ eV

