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Machine-learning quantum transport signatures in 2D materials

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Introduction

Graphene[1] and other 2D materials are very appealing for nanoelectronics, since they could play crucial roles in future nanodevices. At the nanoscopic scale, geometrical effects can critically affect electronic, magnetic, and transport properties[2]. However, disorder in the lattice structure, derived from either defects or external impurities, is extremely difficult to completely eliminate, and can lead to substantial changes in the properties of these systems. Therefore, characterising the effects of realistic disorders on device behaviour remains crucially important.

Theoretical predictions of large-scale disordered systems can be costly, considering the computational resources required to deal with increases in system size. Machine learning techniques have been employed in various fields, such as consumer recommendation systems, aeronautics and chemistry, to exploit patterns in data and make predictions.

Efficient description of disordered systems leads to better prediction for ML techniques. Based on the success of the Couloumb Matrix descriptor alongside Kernel Ridge regression technique in chemical properties[3] and quantum transport prediction[4], we employ a new descriptor, encoding the distance of the impurities from the same sublattice edge[5] and its variants, leading to great prediction performance. These developed techniques can be used to accurately estimate transmission profiles in disordered graphene nanoribbons (GNRs)

Methods & Workflow

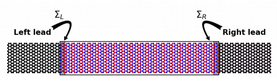
Framework : Tight-Binding Hamiltonian + Recursive Green Function Method

$$\hat{\mathcal{H}} = \sum_{<i,j>} t_{ij} |i\rangle \langle j| + \sum_i \varepsilon_i |i\rangle \langle i| \qquad \hat{g}^{a/r}(E) = \lim_{\eta \to 0} \left[(E \pm i\eta)\hat{I} - \hat{\mathcal{H}} \right]^{-1}$$

1)Quantum Transport :

Generation of disordered systems with 5 impurities : $\epsilon_{\text{impurity}} = 2|t_{ij}|$ with $t_{ij} = -2.7$ eV

Dataset :10000 random disordered configurations
For each configuration :
- Configuration file : Structural defects information
  - X and Y coordinates
  - Sublattice information
  - Indices
- Transmission curve from 0 to 2 eV: Tbtrans/Sisl[6]



$$T_{RL}(E) = Tr\left[\Gamma^L G^r_{LR} \Gamma^R G^a_{RL}\right]$$

Training Set : 8000 configurations
- Model Training :
  - Model selection
  - Hyperparameters research

Test Set : 2000 configurations
Model assessment :
- Mean Absolute error

$$MAE = \frac{1}{n}\sum_n |T^{pred} - T^{ref}|$$

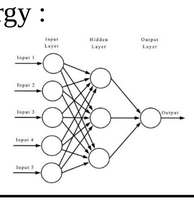
- **Machine Learning:** ⟶ Goal : To predict **transmission** with **geometrical** information

- **Laplacian Kernel ridge Regression (KRR):**
  - Shown promising results in quantum chemistry[3]
  - For each energy :

$$T^{\text{pred}}(E, \mathbf{D}_j) = \sum_{I=1}^{N_t} \alpha_I(E) e^{\left(-\frac{1}{\sigma}|\mathbf{D}_i - \mathbf{D}_j|\right)} \qquad \alpha = [\mathbf{K} + \lambda \mathbf{I}]^{-1} T^{\text{ref}}(E)$$

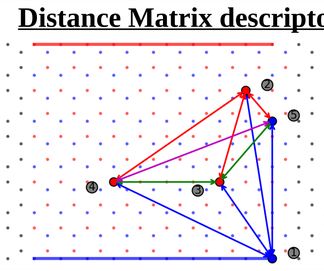
Kernel matrix : $\mathbf{K_{ij}} = e^{\left(-\frac{1}{\sigma}|\mathbf{D}_i - \mathbf{D}_j|\right)}$

- **Neural Network (NN):**
  - For all energy :

Geometrical information + Energy →  → Transmission

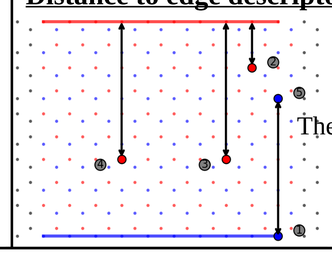
How to infer transmission with geometrical information : The crucial role of Descriptor

Distance Matrix descriptor : DMAT[4]



List of sorted inter-impurity distances
-
Similar to Coulomb Matrix (see Triup)

Distance to edge descriptor : D2E



List of sorted distances :
The distance is taken as the closest **same** sublattice edge

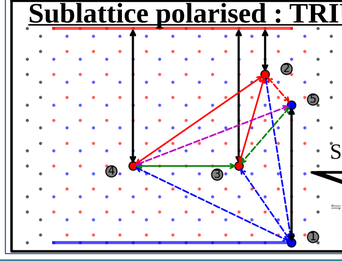
Triangular upper matrix descriptor : TRIUP

TRIUP = D2E + DMAT

$$\leftrightharpoons \begin{pmatrix} d_1 & d_{1-2} & d_{1-3} & d_{1-4} & d_{1-5} \\ 0 & d_2 & d_{2-3} & d_{2-4} & d_{2-5} \\ 0 & 0 & d_3 & d_{3-4} & d_{3-5} \\ 0 & 0 & 0 & d_4 & d_{1-5} \\ 0 & 0 & 0 & 0 & d_5 \end{pmatrix} \leftrightharpoons$$

List of elements sorted and arranged gathering distance to edge
+
inter-impurity informations

Sublattice polarised : TRIUP_SUBPOL



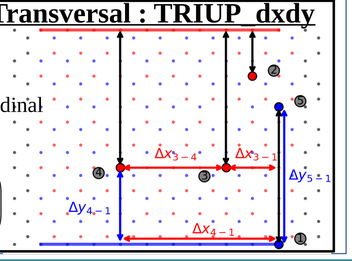
TRIUP_SUBPOL
=
TRIUP
+
Sublattice information

$$\equiv \begin{pmatrix} d_1 & -d_{1-2} & -d_{1-3} & -d_{1-4} & d_{1-5} \\ 0 & d_2 & d_{2-3} & d_{2-4} & -d_{2-5} \\ 0 & 0 & d_3 & d_{3-4} & d_{3-5} \\ 0 & 0 & 0 & d_4 & -d_{1-5} \\ 0 & 0 & 0 & 0 & d_5 \end{pmatrix}$$

Longitudinal/Transversal : TRIUP_dxdy

TRIUP_dxdy
=
Transversal/Longitudinal inter-impurity information

$$\begin{pmatrix} d_1 & \Delta x_{1-2} & \Delta x_{1-3} & \Delta x_{1-4} & \Delta x_{1-5} \\ \Delta y_{2-1} & d_2 & \Delta x_{2-3} & \Delta x_{2-4} & \Delta x_{2-5} \\ \Delta y_{3-1} & \Delta y_{3-2} & d_3 & \Delta x_{3-4} & \Delta x_{3-5} \\ \Delta y_{4-1} & \Delta y_{4-2} & \Delta y_{4-3} & d_4 & \Delta x_{4-5} \\ \Delta y_{5-1} & \Delta y_{5-2} & \Delta y_{5-3} & \Delta y_{5-4} & d_5 \end{pmatrix}$$



Results

1) Small system : 10-ZGNR repeated 10 times

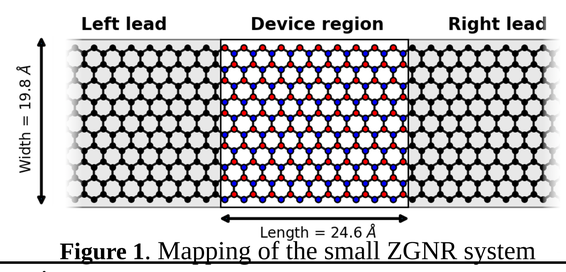


Figure 1. Mapping of the small ZGNR system

- Discussions :
  - KRR and NN results for the DMAT & D2E suggest that the **distance to the same sublattice edge** is the most relevant information to characterize disordered GNRs.
  - Combining D2E & DMAT alongside with additional informations such as **impurity sublattice dependency** or **transversal/longitudinal inter-impurity** distance improves the predictive power of NN techniques.

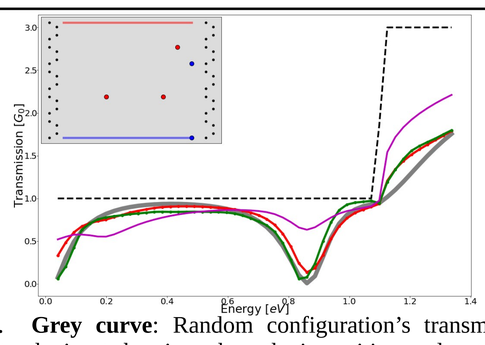


Figure 3. **Grey curve**: Random configuration's transmission from unseen data, the inset showing where the impurities are located.
Black dotted line – purple curve : Pristine transmission – averaged transmission.
Red curve: Prediction with D2E alongside with NN.
Green curve : Prediction with TRIUP_dxdy alongside with NN.

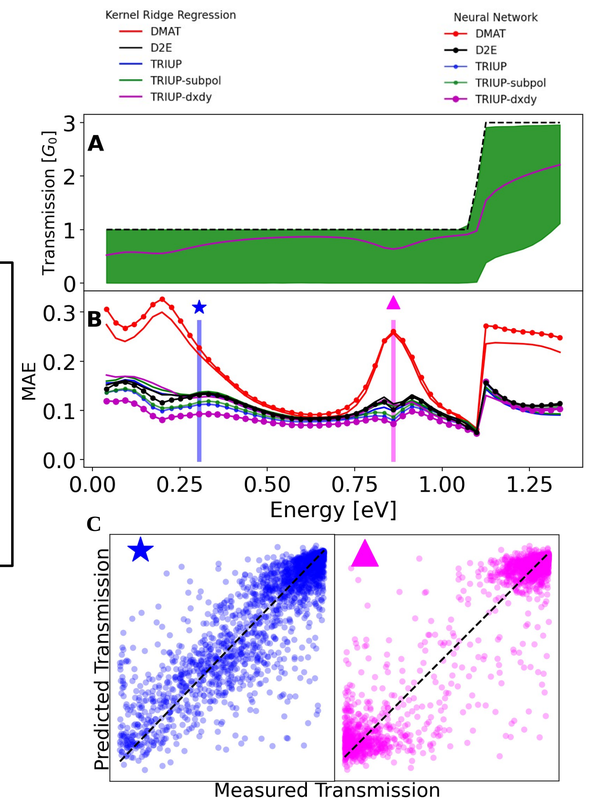


Figure 2. **A –** Training set transmission curve distribution. The dashed black line accounts for the pristine ribbon's transmission and the purple curve for the average transmission in the training set.
B – MAE vs E for all the descriptors, solid lines display KRR results whereas dotted lines stand for NN results.
C – Prediction vs measured transmission for the test set at 2 different energies performed with the best descriptor TRIUP_dxdy with NN.

2) Big system : 18-ZGNR repeated 52 times

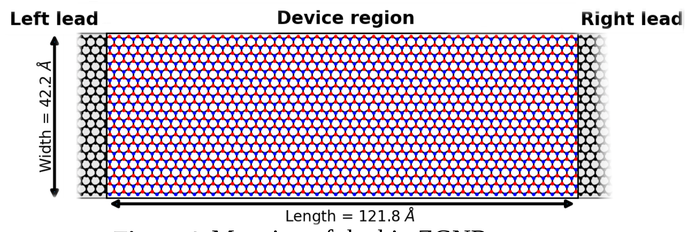
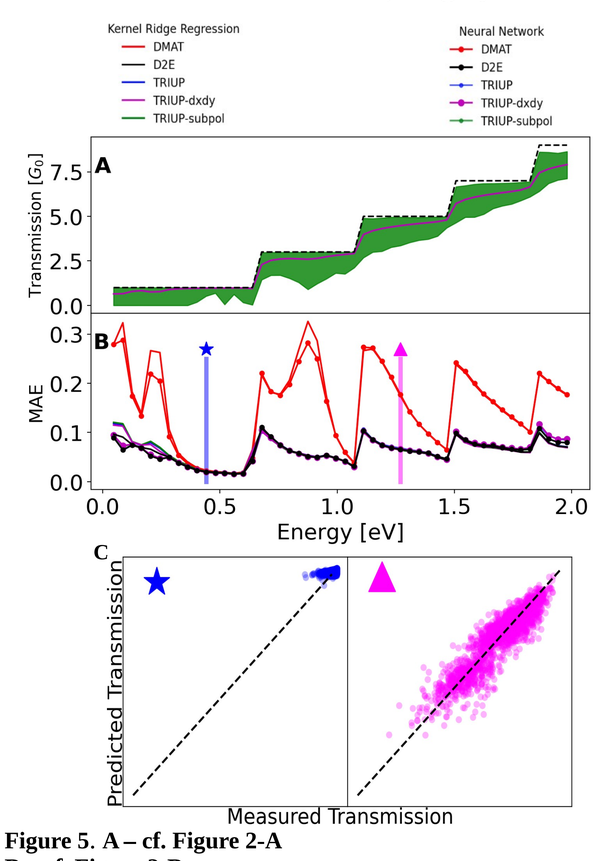


Figure 4. Mapping of the big ZGNR system



- Discussions :
  - As the system gets wider, the distance to the same sublattice edge remains the most crucial information.
  - Additional informations given as input for either KRR or NN techniques do not lead to better performance, emphasizing how important **D2E** is to characterize impurity-based disordered in quasi 1-dimensional systems.

Figure 5. **A – cf. Figure 2-A**
B – cf. Figure 2-B
C – Prediction vs measured transmission for the test set at 2 different energies performed with the best descriptor TRIUP_SUBPOL with NN

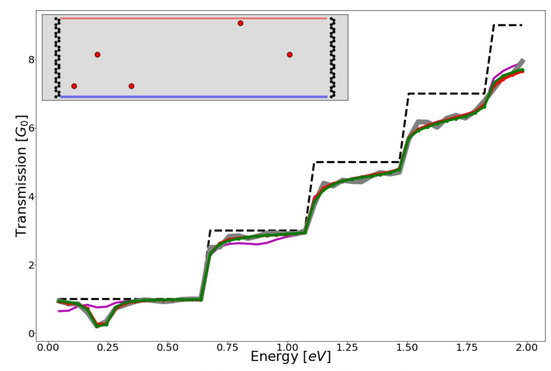


Figure 6. **cf Figure 3**

Conclusions

An approach based on ML techniques to predict electronic transport in disordered nanostructures in complement of the usage of conventional techniques has been presented. By implementing ML techniques such as KRR or NN on a generated dataset, it has been shown that one can perform computations that will have a moderate cost in comparison of system-scaled conventional techniques.

In both cases, a careful choice of descriptors greatly improves the performance of the ML techniques. We have shown that descriptors can be improved by taking into account local sublattice and edge effects, which can dominate over impurity separation. The information encoding the distance of the impurities to the same sublattice edge in ZGNR revealed to be crucial to describe efficiently quasi-one-dimensional system subject to disorder. Our results highlight the ability of ML techniques to capture the complexity of disordered nanostructures, and suggest that they can be used to complement conventional techniques to better understand a wider array of systems.

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