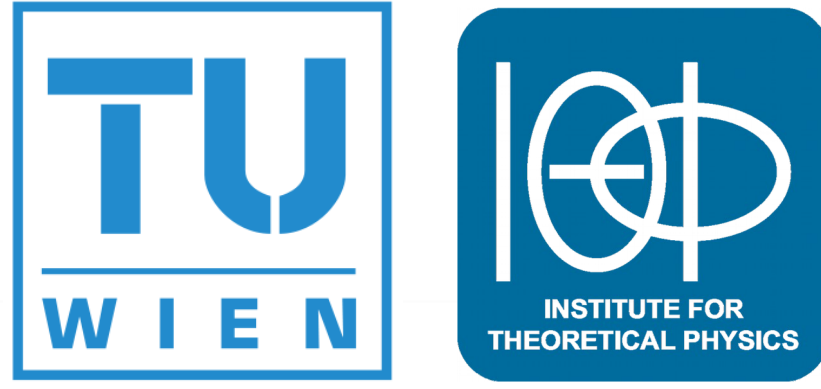


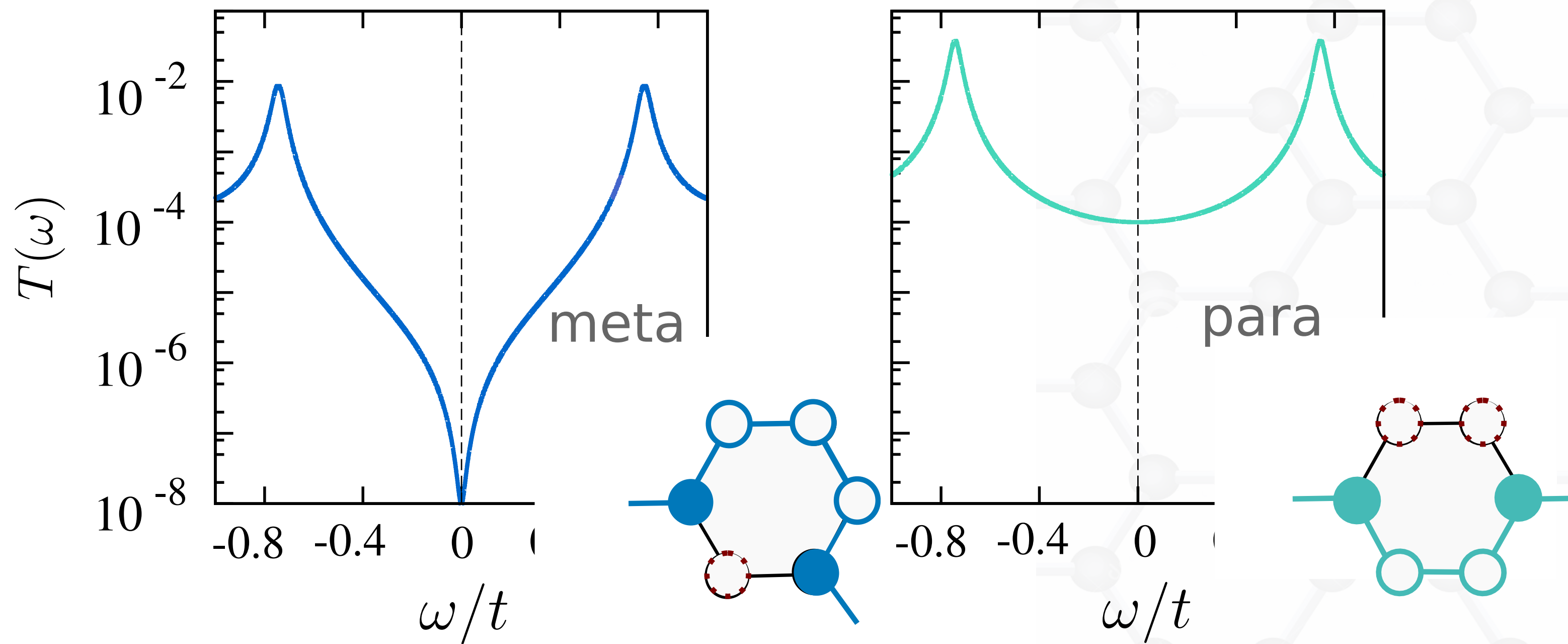
## DESTRUCTIVE QUANTUM INTERFERENCE IN GRAPHENE-LIKE SINGLE MOLECULE JUNCTIONS



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### Destructive Quantum Interference (DQI)

- New paradigm for logic devices based on GNRs with extremely low power consumption
- A tool for increasing the selectivity of GNR-based gas sensors GNR nanopores and used for DNA base sequencing

Transmission function  $T(E)$ :

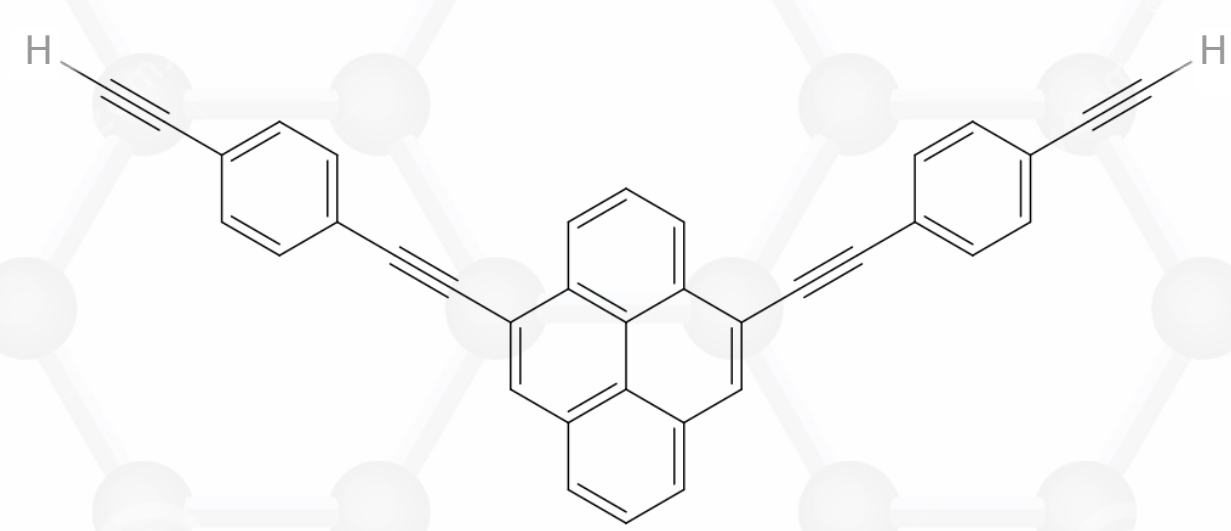
$$T(E) = \text{Tr}[G^r(E)\Gamma_L(E)G^a(E)\Gamma_R(E)]$$

### aim of this work

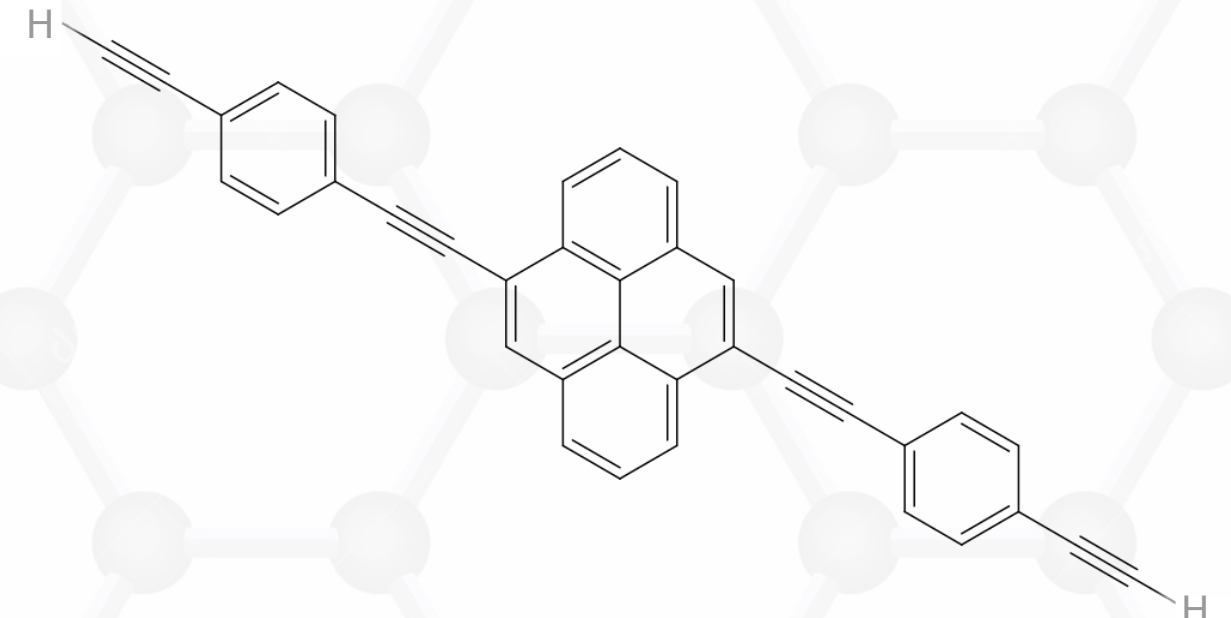
Acetylene anchor group with linkers at meta- or para-positions are studied to assess the structure-function relationship of molecular junctions with different connectivities to probe electronic transport features and **DQI effects**. Graphene leads topology can influence the shape of the transmission

### ELECTRON-TRANSPORT CALCULATIONS

The thiol-terminated anchor units are identified as 4,10-pyrene and 5,10-pyrene based on to the connectivity to the central pyrene.

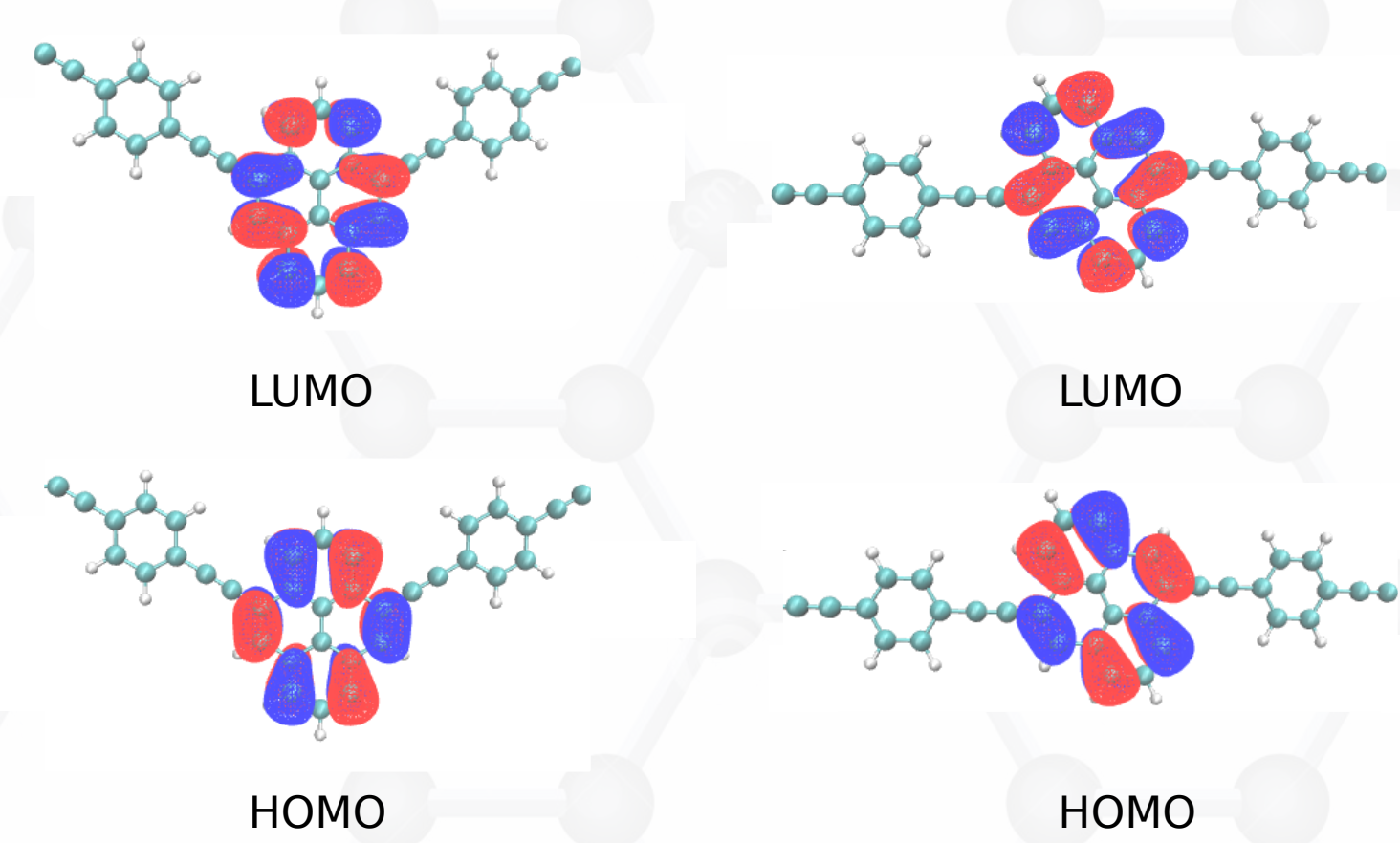


4,10-pyrene → DQI



5,10-pyrene → no DQI

### Molecular orbitals of zigzag edge graphene



Gold electrodes have the same representation for the frontier orbitals

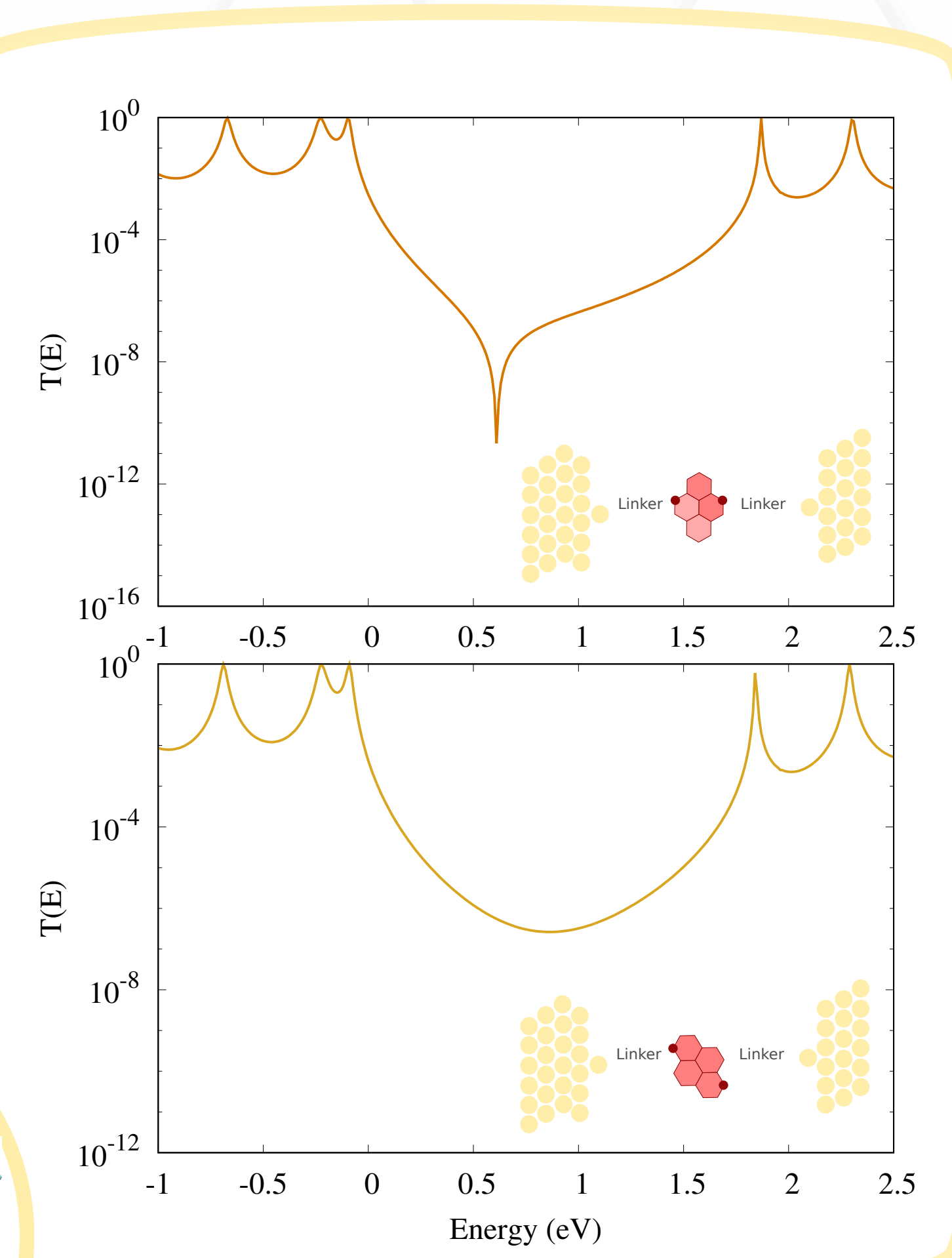
4,10-pyrene has destructive interference and 5,10-pyrene has constructive interference

DQI can also be understood from the analysis of frontier molecular orbitals, with:

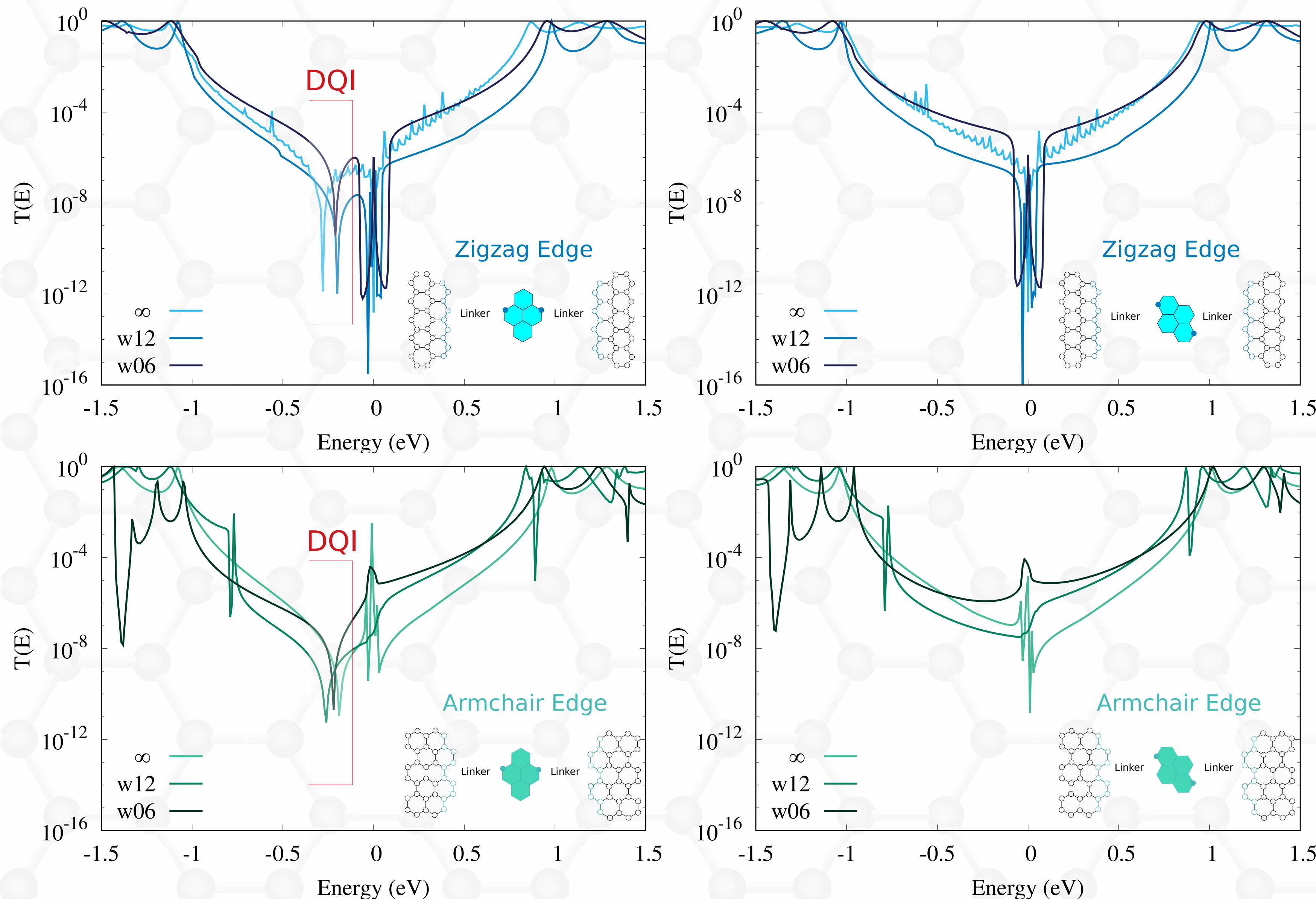
$$G_{lr}^{mol}(E) = \sum_{m=1}^N \frac{C_{lm}C_{rm}^*}{E - \epsilon_m \pm i\eta}$$

And the simplified form as Larsson's formula

$$\Gamma(E) = \sum_{m=1}^N \frac{\alpha_m \beta_m}{E - \epsilon_m}$$

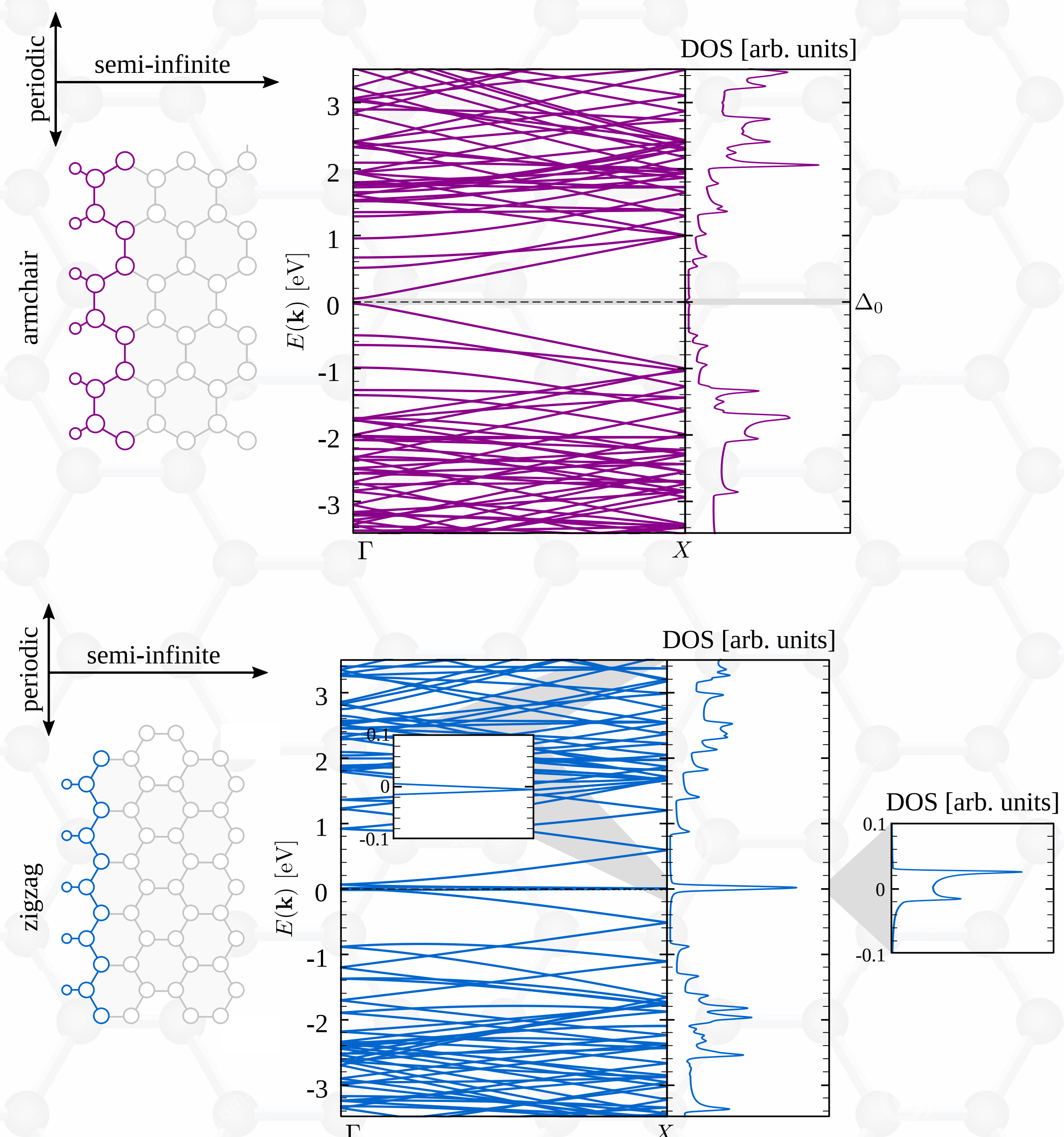


Transmission Function of molecules in between Gold leads and Schematics of Single-Molecule Junctions



Transmission Function of Graphene leads with different edge shapes, namely, zigzag and armchair and varying edge lengths ( $W=6$ ,  $W=12$ ,  $W=\infty$ ) with Schematics of Single-Molecule Junctions

### Density of States (DOS)



### Computational Details

- $T(E)$  is performed within a NEGF-DFT framework with the GPAW code.  
- Electron-transport and electron-structure calculations: LCAO (DZP).

### REFERENCES

- [1] O. Sengul, A. Valli, and R. Stadler, in preparation (2020).
- [2] Zhao *et al* J. Chem. Phys., 092308 (2017)
- [3] Markussen *et al*, Nano Lett. 2010, 10, 10, 4260-4265