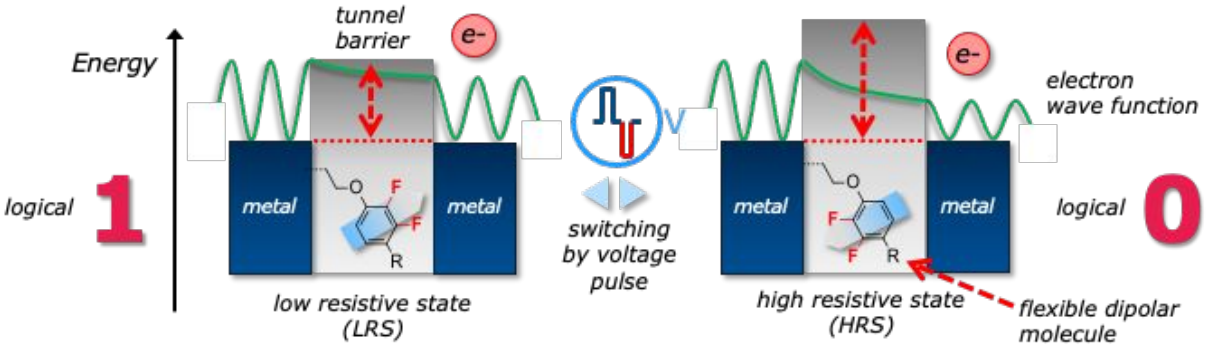
Modelling IV characteristics of FTJ

Case Study performed by Prof. Dr. Peer Kirsch (Technische Universität Darmstadt) based on: J. Dlugosch, H. Seim, A. Bora, T. Kamiyama, I. Lieberman, F. May, F. Müller-Plathe, A. Nefedov, S. Prasad, S. Resch, K. Saller, C. Seim, M. Speckbacher, F. Voges, M. Tornow, P. Kirsch, "Conductance Switching in Liquid Crystal-Inspired Self-Assembled Monolayer Junctions", ACS Appl. Mater. Interfaces 2022, 14, 31044-31053 (doi: 10.1021/acsami.2c05264)

Model system: A ferroelectric tunnel junction (FTJ), which is based on a self-assembled monolayer (SAM) of small, functional molecules.



Schematic representation of the fundamental principle: the conformationally flexible dipole of the FTJ can be reversibly reoriented in an electrical field. The SAM acts as an electrically switchable tunnel barrier.

Potential application in the field of information storage and processing, in particular for in-memory and neuromorphic computing architectures.

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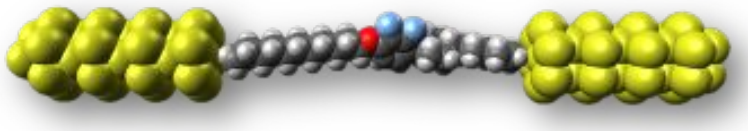
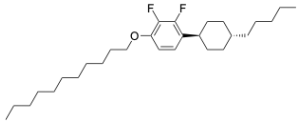
The computational IV characteristics of Au/SAM/Au were computed by using the electronic transport workflow implemented in ASAP.



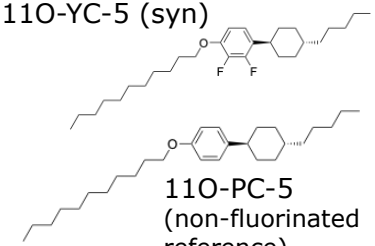
ASAP builder creates ball-and-stick model representation of the junction layout.

Considered conformers:

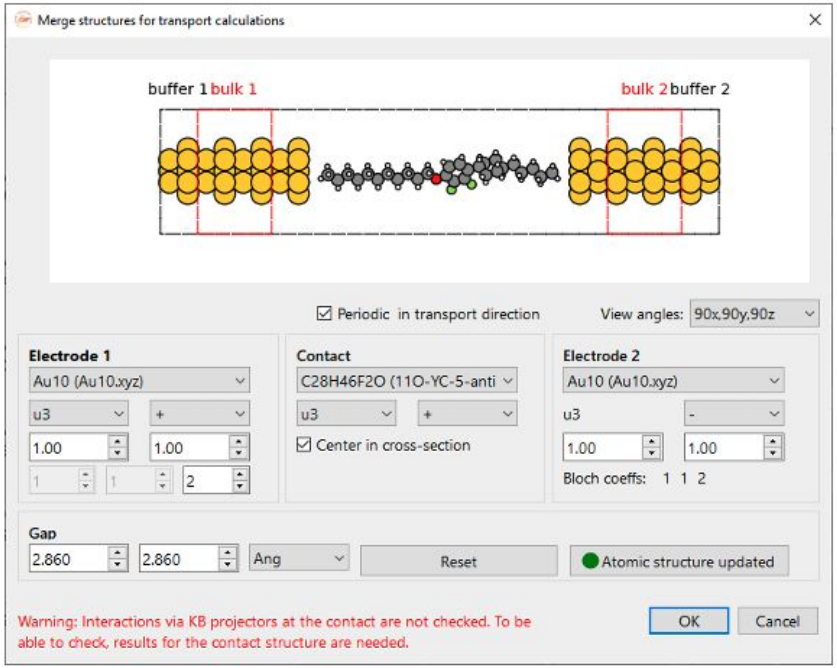
11O-YC-5 (anti)



11O-YC-5 (syn)



11O-PC-5
(non-fluorinated reference)

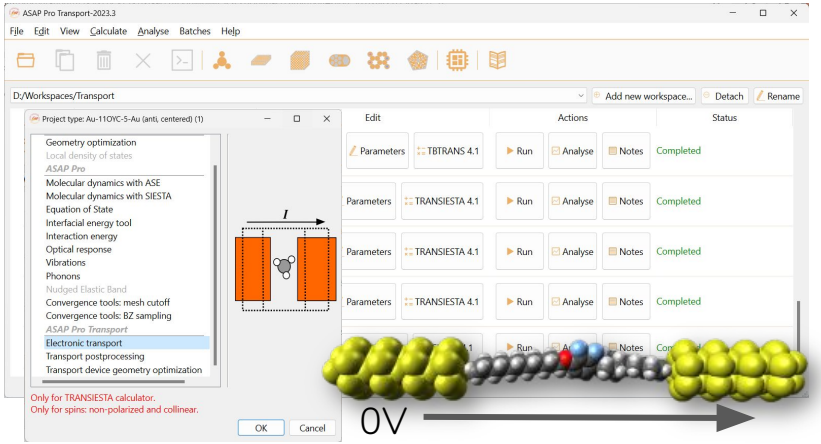


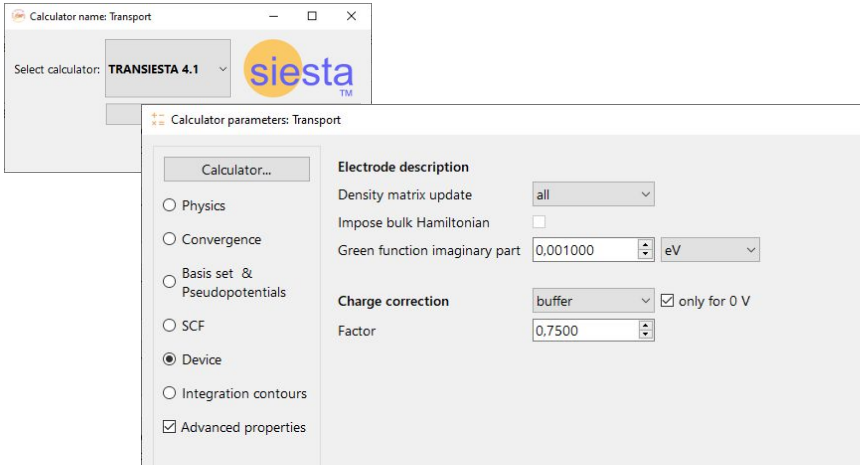
Screenshot of junction setup builder in ASAP

Modelling IV characteristics of FTJ

ASAP's user-friendly graphical interface was used to input parameters for the TranSIESTA code[1].
A series of transport calculations were carried out by incrementally applying higher voltages* to the system (automated workflow in ASAP).

*The voltage is applied to the system along the transport direction.





We used the pseudopotentials and corresponding basis sets provided by ASAP.
https://www.simuneatomistics.com/siesta-pro/siesta-pseudos-and-basis-database/

[1] N. Papior, et al Comp. Phys. Comm. 212, 8 (2017)

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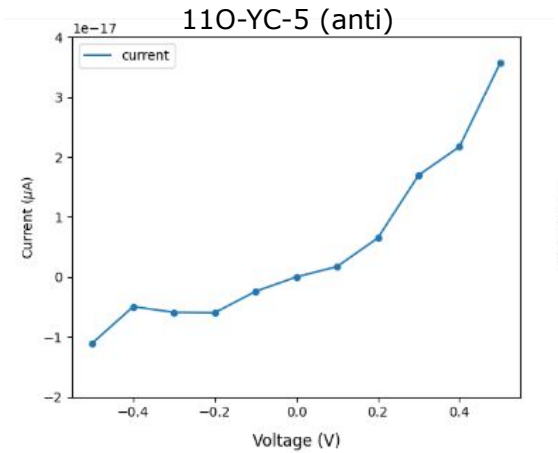
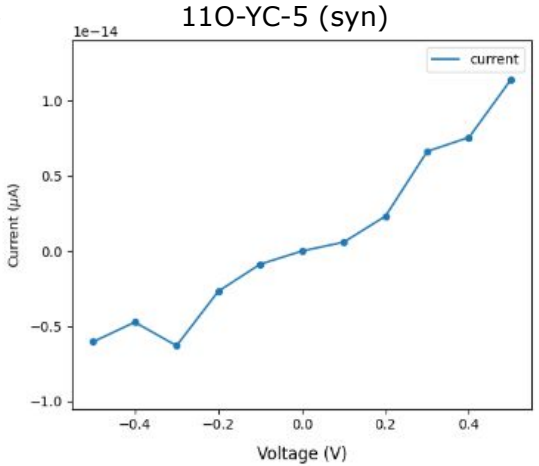
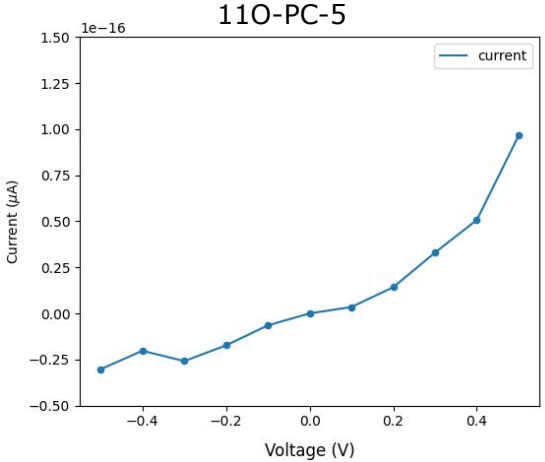
ASAP Transport post processing workflow was used to compute and visualise the current-voltage curves of the considered Au/SAM/Au junctions.







- *syn* conformer shows similar conductance as non-fluorinated reference
- the I-V curve is conformational dependent, an effect previously reported for similar molecules. (J. Dlugosch et al. ACS Appl. Mater. Interfaces 2022, 14)

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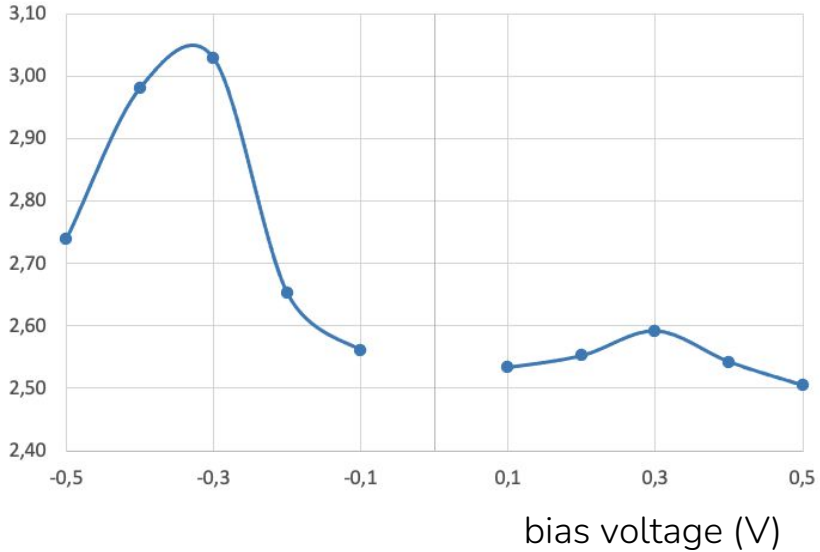
Computational IV Characteristics

- switching between *anti* and *syn* conformers causes conductance change (memory window) of 2.5-3.1 orders of magnitude
- memory window shows maximum at -0.3 V

Memory window $\log_{10}(I_{syn}/I_{anti})$



Request a trial version of ASAP.

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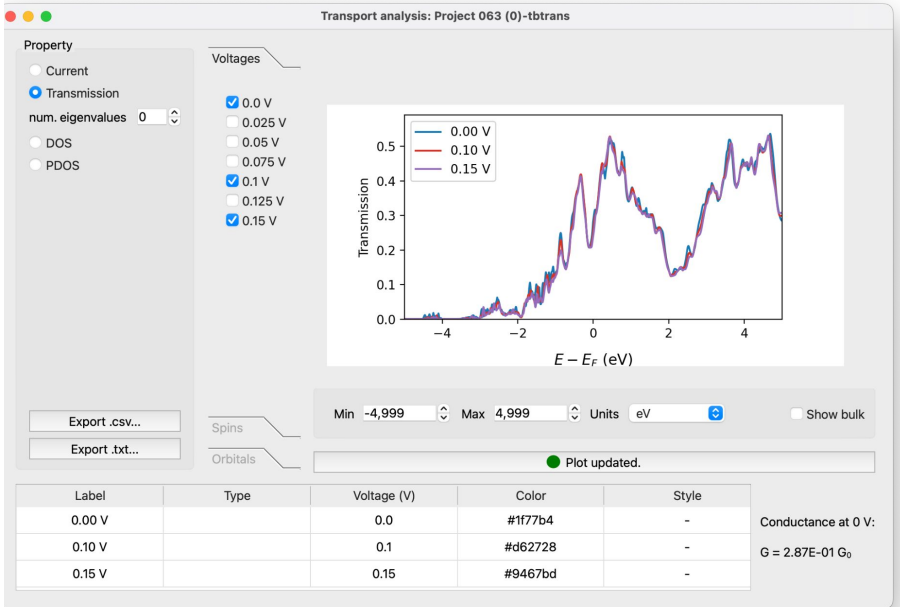

ASAP analysis window showing the transmission at different voltages. The conductance at 0V is obtained from the transmission spectra.

We predict a conductance (G_{Cu}/water-molecule/$_{GCu}$) at 0 V to be 0.197 G0.