

Case Study performed by <u>Prof. Dr. Peer Kirsch</u> (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.

www.simuneatomistics.com



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:



	buffer 1	bulk 1	-0		bulk 2 buffer 2		
				<u>~~~</u> ??????		\$ \$9	
ectrode 1			✓ Periodic Contact	in transport direction	Electrode 2	gles: 90x,90y,90z	
ectrode 1 Au10 (Au10	xyz)	~	Periodic Contact C28H46F2O (in transport direction	Electrode 2 Au10 (Au10.)	gles: 90x,90y,90z	
lectrode 1 Au10 (Au10 13	xyyz) + 1.00	~	Periodic Contact C28H46F2O (U3 ~ Center in cr	in transport direction	Electrode 2 Au10 (Au10.) u3	gles: 90x,90y,90z	
lectrode 1 Au10 (Au10) u3 1.00	xyz) + 1.00 2	>	 ✓ Periodic Contact C28H46F2O (u3 ~ ✓ Center in cr 	in transport direction	Electrode 2 Au10 (Au10.) u3 1.00	gles: 90x,90y,90z	
Iectrode 1 Au10 (Au10 u3 1.00	xyz) v + 1.00 \hat{v} 2	>	 ✓ Periodic Contact C28H46F2O (u3 ~ ✓ Center in cr 	in transport direction 110-YC-5-anti v + v oss-section	Electrode 2 Au10 (Au10.3 u3 1.00 Bloch coeffs:	gles: 90x,90y,90z xyz) ~ - ~ 1.00 * 1.1 2	

Screenshot of junction setup builder in ASAP



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.

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D:/Workspaces/Transport		×][Add new workspace Detach Add new workspace	Calculator parameters: Tran	sport	
Project type: Au-110YC-5-Au (anti, centered) (1) Geometry optimization Local density of states solar Days of states	× Edit Parameters TBTRANS 4.1	Actions	Status Notes Completed	Calculator	Electrode description	×
Molecular dynamics with ASE Molecular dynamics with SIESTA Equation of State <u>I</u> Interfacial energy tool <u>I</u>	Parameters TRANSIESTA 4.1	► Run Analyse	Notes Completed	O Physics O Convergence	Impose bulk Hamiltonian Green function imaginary part	0,001000 ≑ eV ∽
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Transport postprocessing Transport device geometry optimization Only for TRANSIESTA calculator. Only for spins: non-polarized and collinear.		99999	Con	 Integration contours Advanced properties 		

We used the pseudopotentials and corresponding basis sets provided by ASAP.

https://www.simuneatomistics.com/siesta-pro/siesta-pseudos-and-basis-database/



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







Request a trial version of ASAP.







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

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