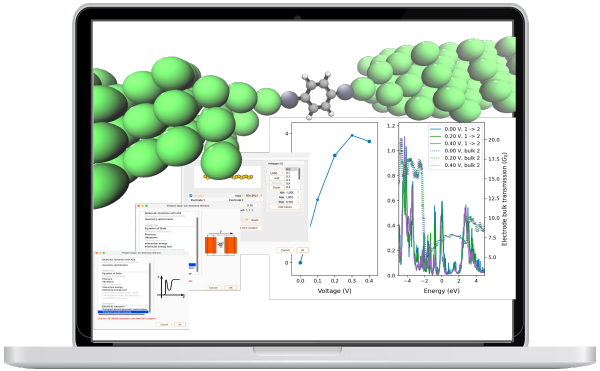
Electronic nano-transport workflow in ASAP

ASAP provides an user-friendly workflow for studying electronic nano-transport

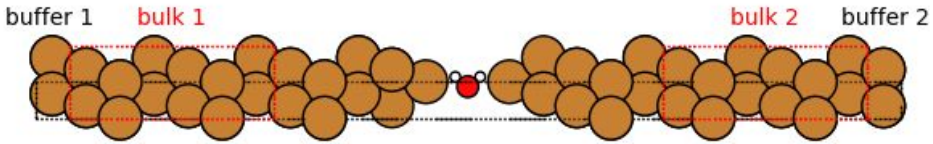


- Fully automated AI supported Device builder
- TranSIESTA-NEGF graphical user interface
- Local and remote task control
- Analysis Tools:
  - Construction and visualisation of planar and macro-average of electrostatic potential across the device
  - Construction transmission function for the device for bulk electrodes
  - Spin resolved plots for transmission and current (including spin difference and spin sum plots)

Case Study: Electronic Current on Cu/water/Cu junction

Single-molecule junctions (SMJs) are attractive structures for developing the reactions enhancing the efficiency of water splitting*.

In this case study, we have employed Atomistic Simulation Advanced Platform (ASAP-Transport) for modelling the transmission spectrum and I-V curve of Cu-based junction, an attractive water-splitting environmental catalysts.

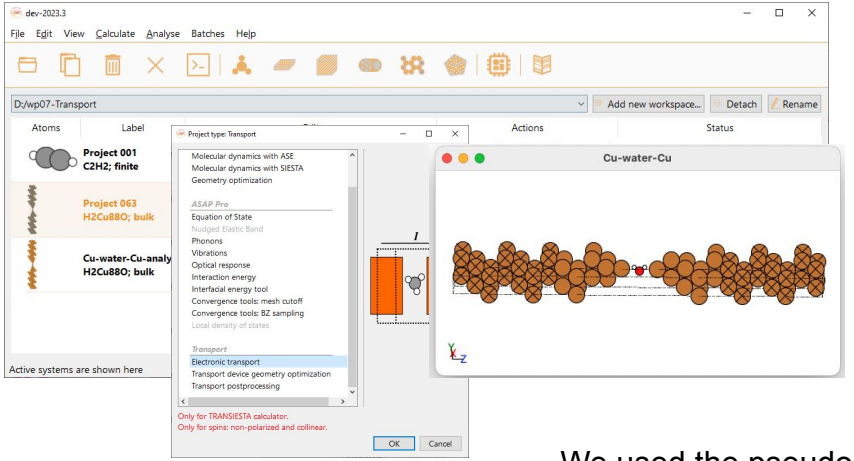


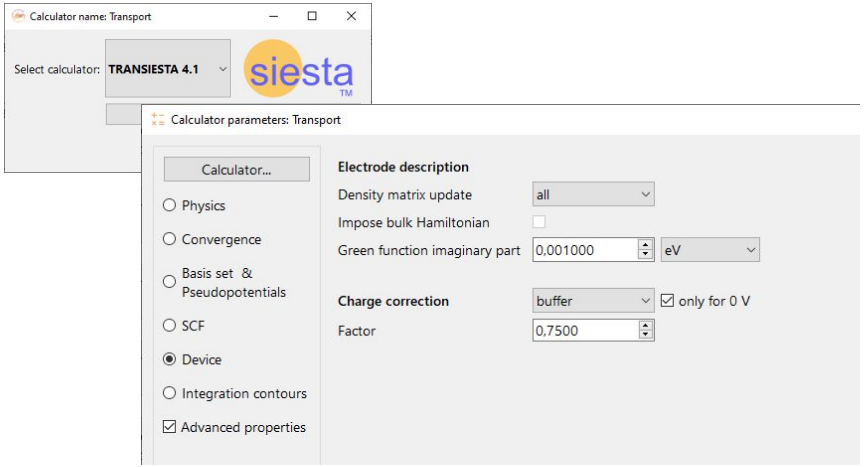
ASAP builder created ball-and-stick model representation of the Cu/water molecule/Cu junction. We considered the atop contact motif for the water molecule

* water splitting refers to the process of breaking water (H_2O) into its two main components; H_2 and O_2. Water splitting, particularly when powered by renewable energy sources, holds great promise for a sustainable energy future and has a wide range of applications across various industries (hydrogen fuel production, energy storage…)

Case Study: Electronic Current on Cu/water/Cu junction

We used ASAP's user-friendly graphical interface to input parameters for the TranSIESTA code[1].
We carried out a series of transport calculations by incrementally applying higher voltages to the system (automated workflow in ASAP).
The voltage is applied to the system along the transport direction.



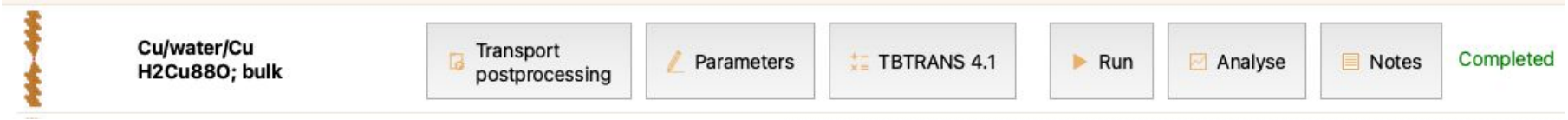


We used the pseudopotentials and corresponding basis sets provided by ASAP.
https://www.simuneatomistics.com/siesta-pro/siesta-pseudos-and-basis-database/

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

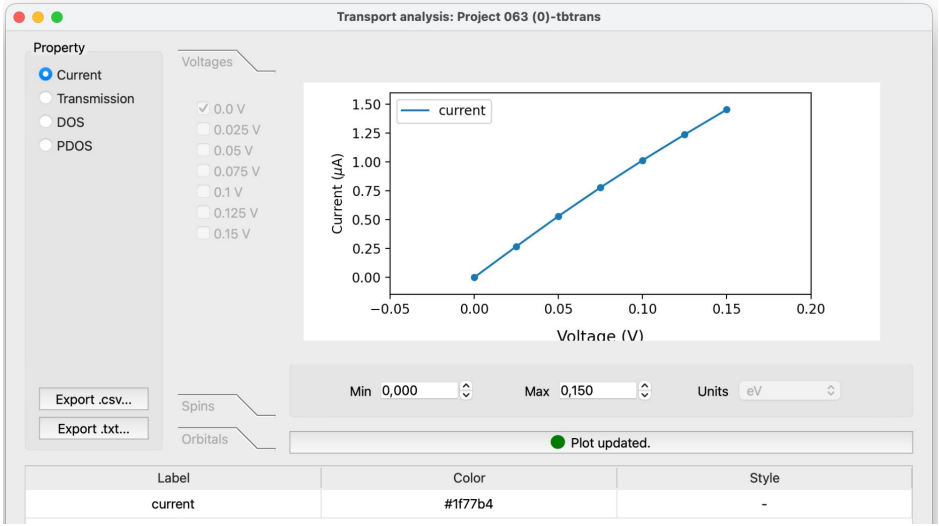
Case Study: Electronic Current on Cu/water/Cu junction

We used ASAP Transport postprocessing workflow to compute and visualise the current-voltage curves and the transmission spectra of the Cu/water molecule/Cu junction.

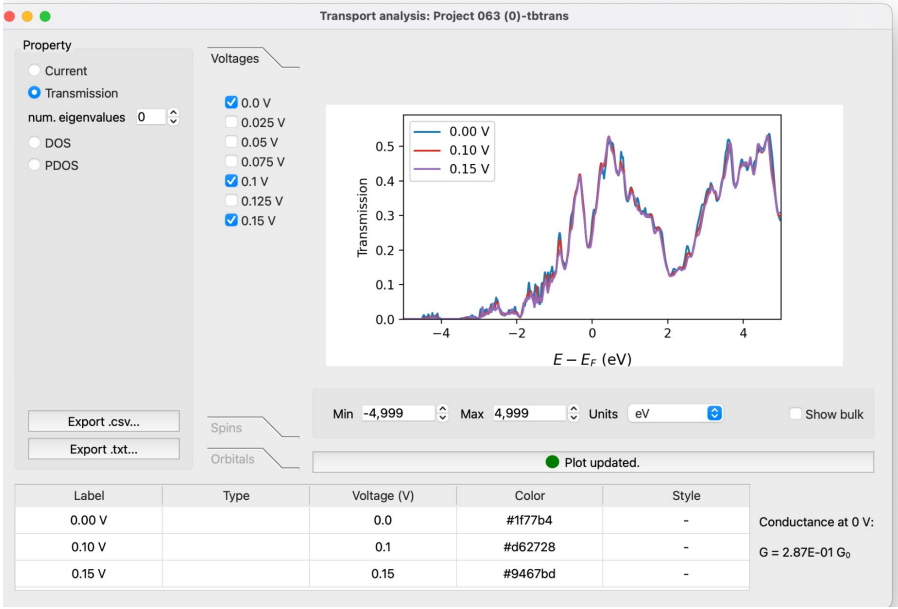


Output:

- Current - Voltage curve
- Transmission (at different voltages)
- DOS and PDOS for electrodes and device
- Spin difference and spin sum plots for current, transmission and transport DOS
- Number of eigenvalues for transmission plot
- Conductance a 0 V



Case Study: Electronic Current on Cu/water/Cu junction



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.

Our results are in agreement with previously reported DFT-based conductance study (R. Fukuzumi, *et al*, Small 17, 2008109 (2021)).