Testcase:
TCAD Simulation of double-layer 2D FTJ

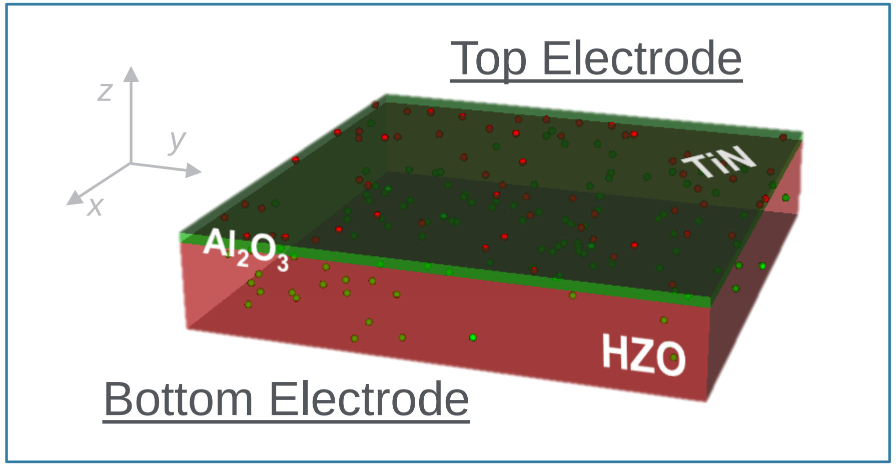
Ginestra® powered

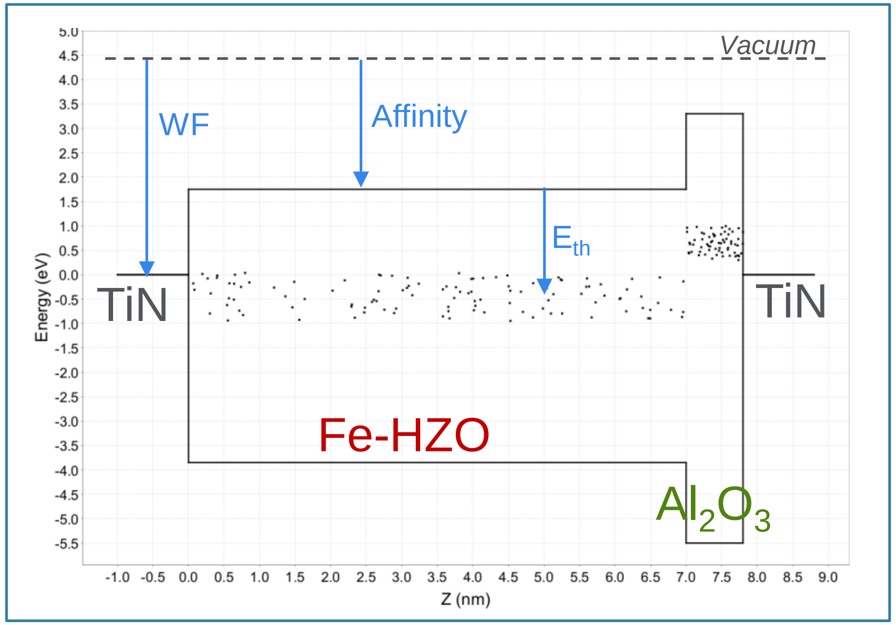
Applied Materials Inc.

APPLIED MATERIALS®
make possible

Device under test: TiN / HZO / AlOx / TiN stack

Tested Ferroelectric-Tunneling-Junction (FTJ) is hereafter described, and its default parameters listed





Parameter	Value used
Geometry	
Al_2O_3 Thickness	0.8 nm
HZO Thickness	7 nm
Width x Length	40nm x 40nm
TiN Properties	
Work Function	4.75 eV
Al_2O_3 Properties	
Permittivity	9.3
Affinity	1.45 eV
Bandgap	8.8 eV
HZO Properties	
Permittivity	25
Affinity	3 eV
Bandgap	5.6 eV
PGL Ferroelectric Parameters	
α	-5.6×10^8 m/F
β	3.1×10^9 $m^5/(FC^2)$
γ	0
ρ	4 kΩm

Defect properties	Value used
Al_2O_3 defects	
Thermal Ioniz. Energy, Eth	2.65 eV
Empty state charge	0 e
Density	5×10^{19} cm^{-3}
HZO defects	
Thermal Ioniz. Energy, Eth	2.2 eV
Empty state charge	0 e
Density	1×10^{19} cm^{-3}

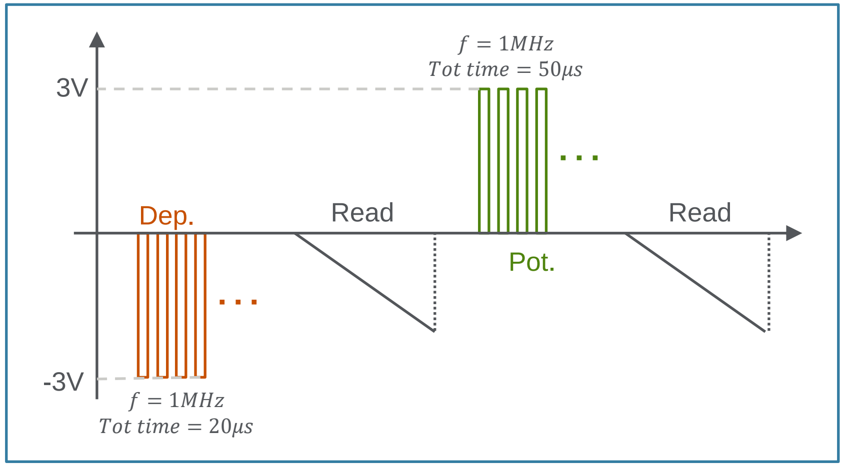
APPLIED MATERIALS

2D Simulation setup

Virtual experiment setup and main physical settings are hereafter reported.

- DoE on TiN work functions is run: WF = [4.65, 4.75, 4.85] eV

- Input signal sequence:
  1. FTJ is depressed with a pulsed scheme at negative voltages
  2. FTJ's current is then read (transient voltage sweep)
  3. FTJ is potentiated with a pulsed scheme at positive voltages
  4. FTJ's current is read again



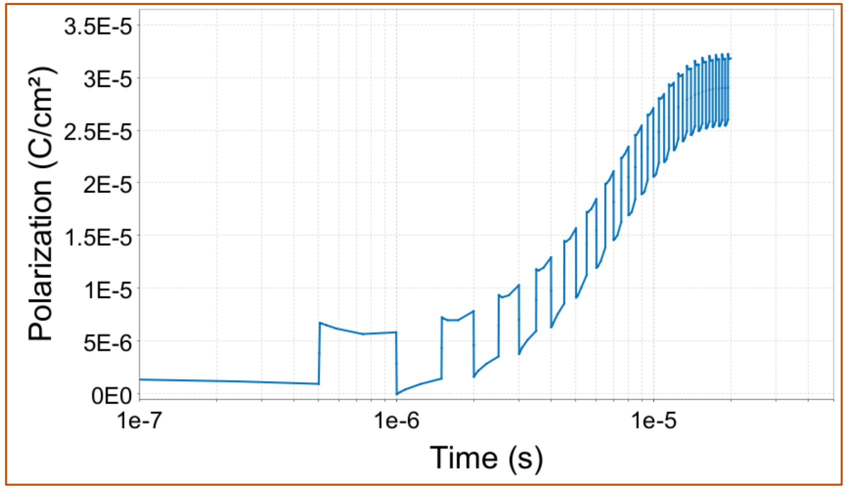
- Physical and Simulation settings:
  - In band transport (Conduction Band)
  - Discrete defect description in dielectrics
  - Full Poisson coupling (defects, ferroelectric polarization)
  - Full dielectric transport (Tunneling, Fowler–Nordheim, Trap-Assisted-Tunneling, Trap-to-Trap)
  - Landau-Ginzburg ferroelectric model (isotropic)
  - Constant temperature: 300K

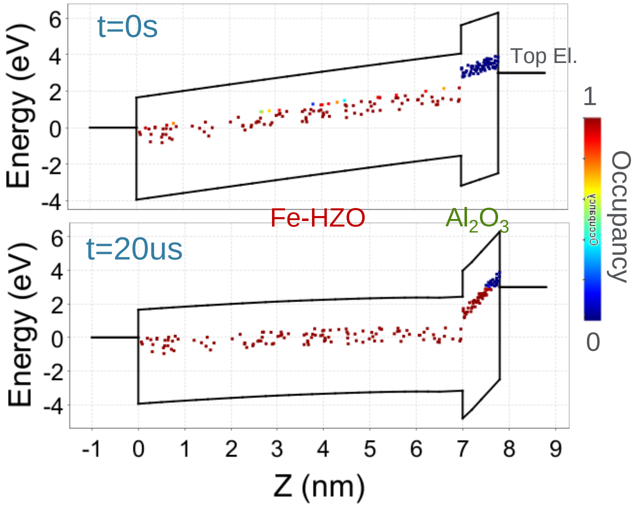
Output results

Ferroelectric behavior during depression and potentiation are reported. Resulting IVs reads are compared.

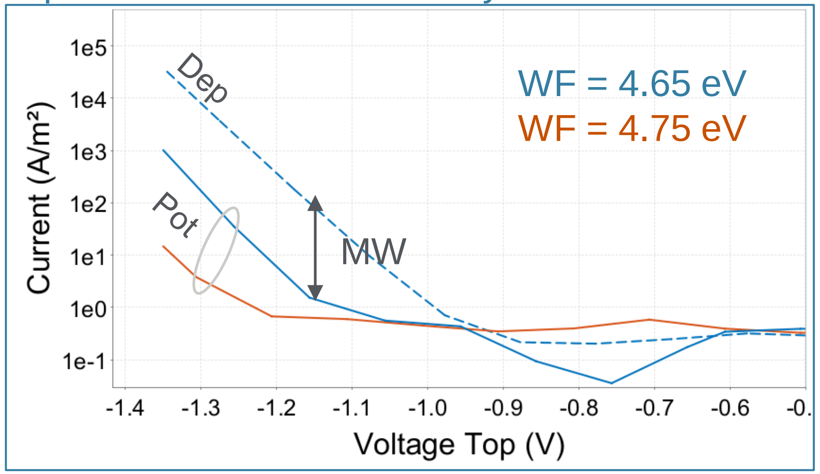
Depression

Av. Ferroelectric Polarization



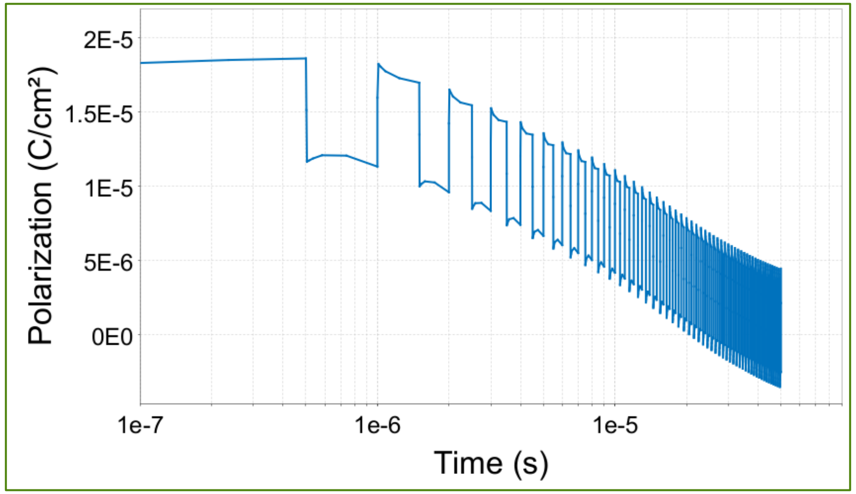


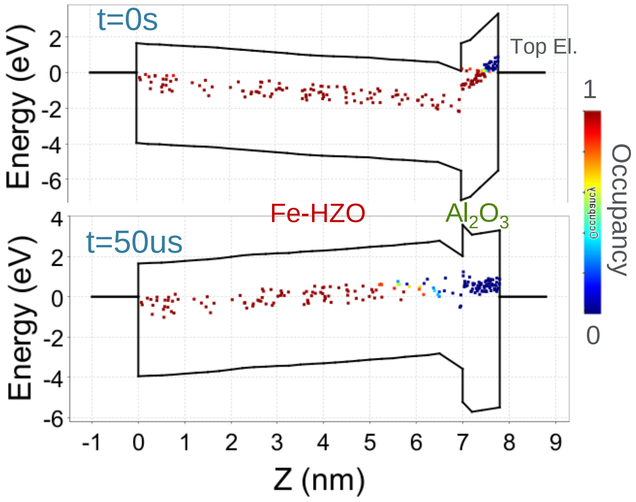
Top Electrode Current Density



Potentiation

Av. Ferroelectric Polarization





- Evident dependance on electrode's WF
- Domains are not all switched at end of potentiation process
- Defects are dynamically interacting with ferroelectric domains and impacting current

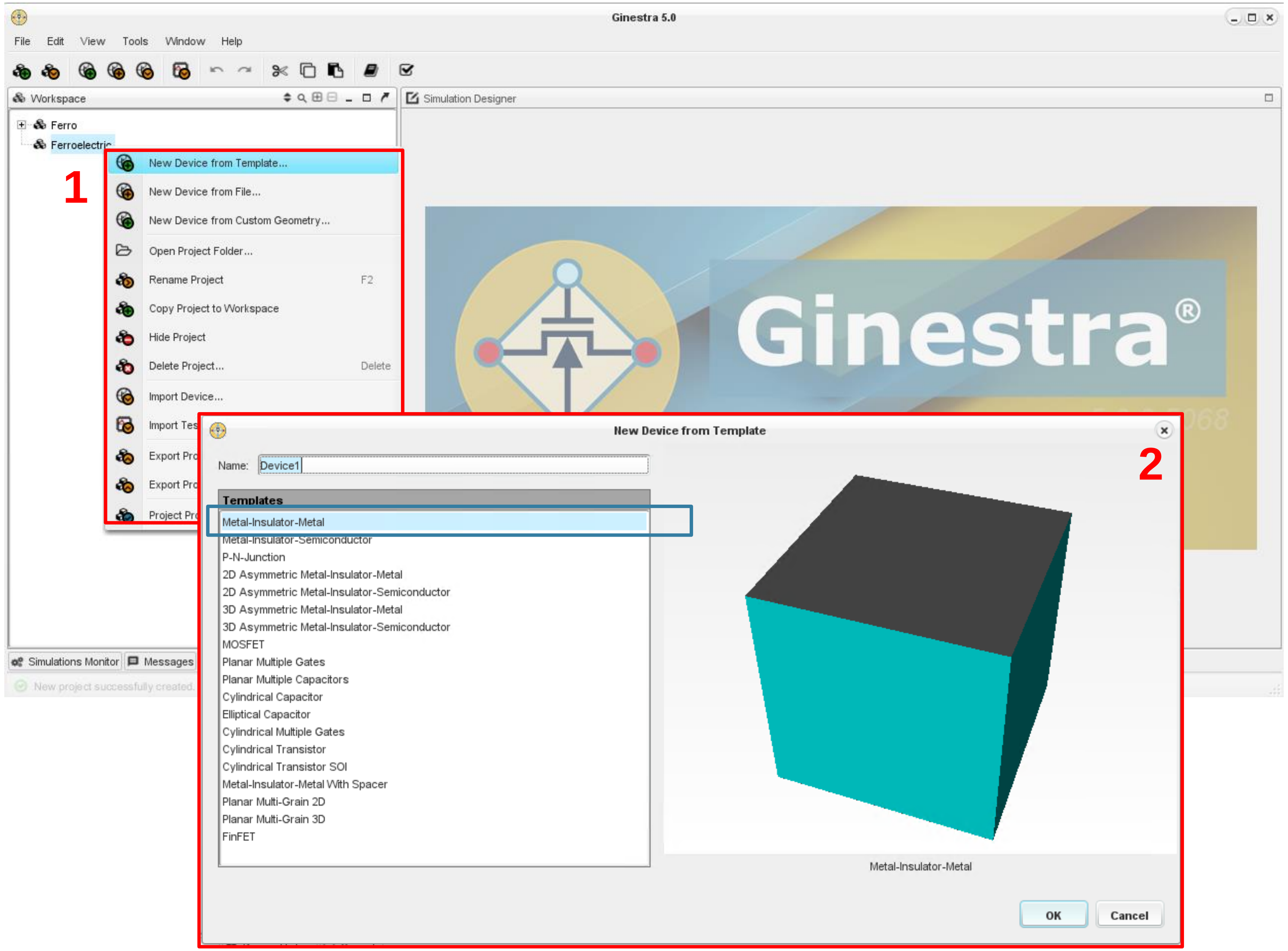
APPLIED MATERIALS

FTJ simulation: HOW TO

with Ginestra® tool

APPLIED MATERIALS®
make possible

1. FTJ: Device creation



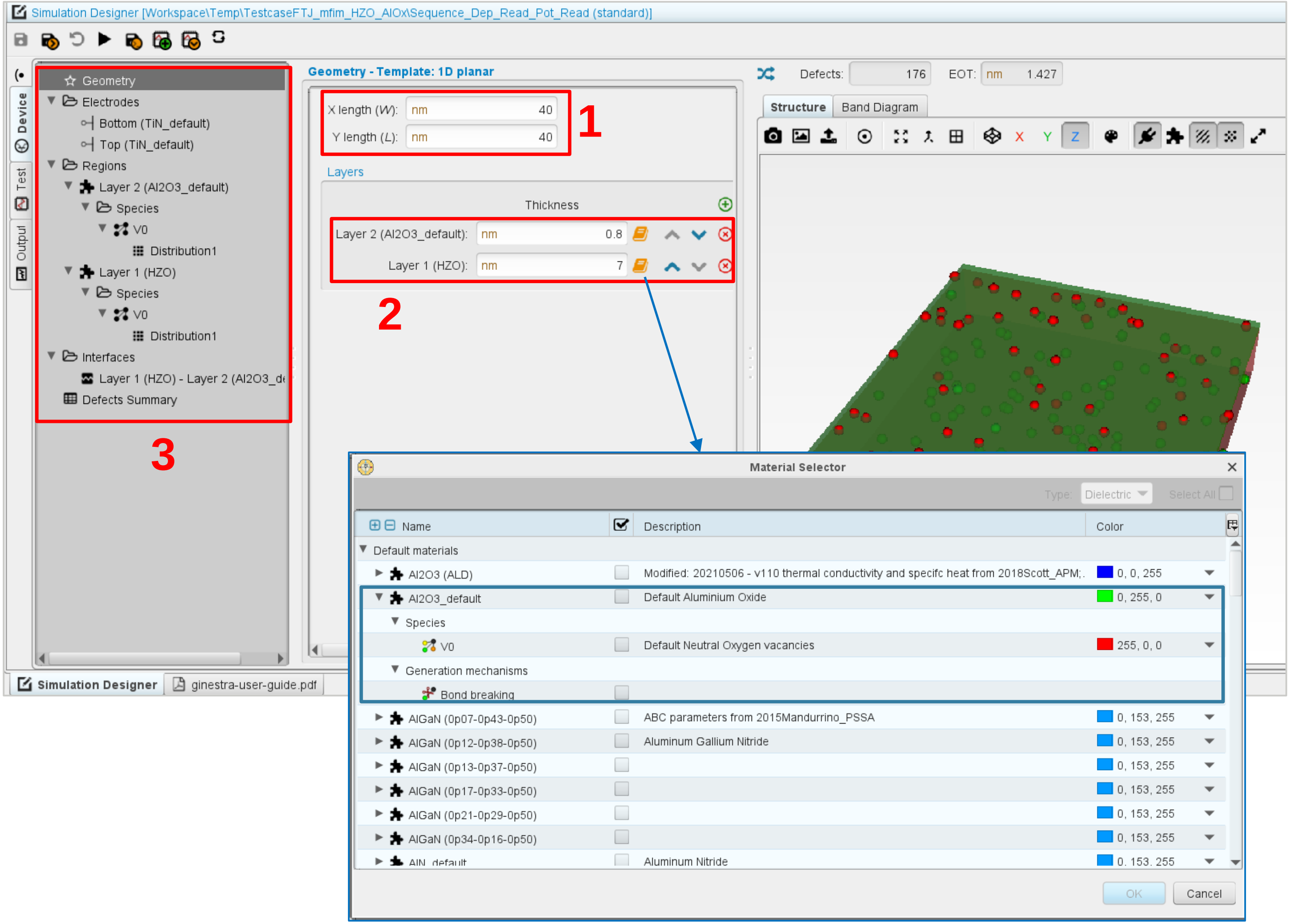
1.1 Device Template

To create a simple double layer FTJ using Ginestra templates:

- (**1**) right-click on the project name and select *New Device From Template*
- (**2**) this will open the *New Device* panel, from which it is possible to select "Metal-Insulator-Metal"

- Note: electrodes can be switched between metallic, semiconductor or ideal.

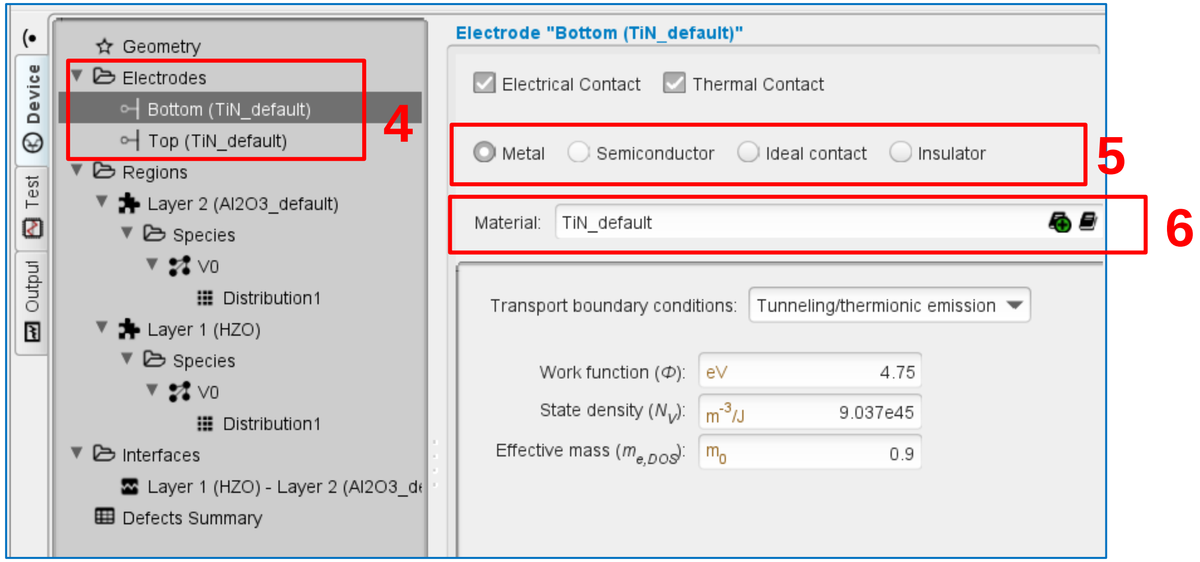
1. FTJ: Device creation

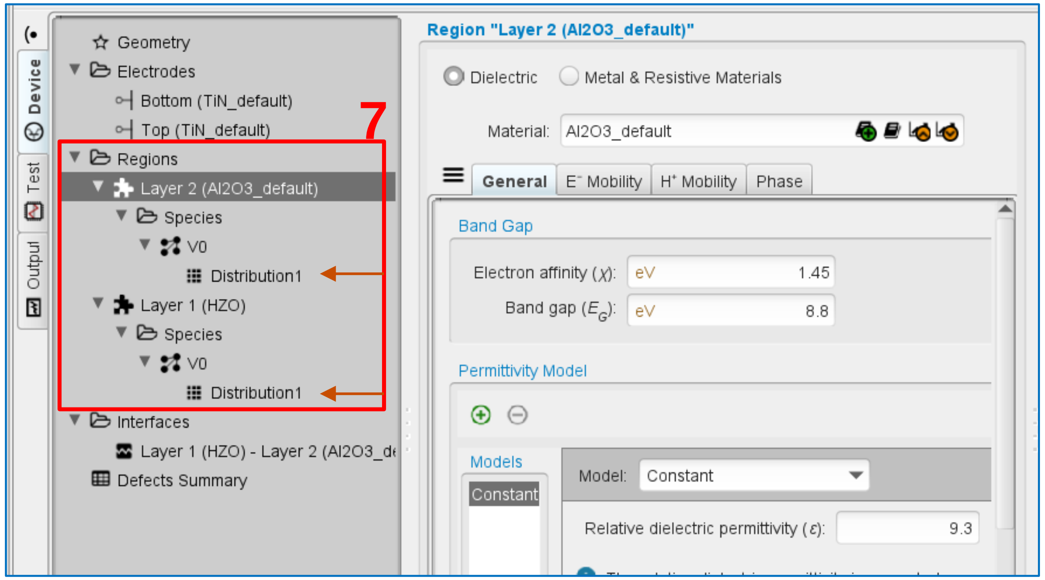


1.2 Stack Composition

- The new device can now be modified.
- (1) The area of the capacitor through (X-length and Y-length parameter).
  - *We set X-length=40nm, Y-length=40nm*
- (2) thickness, stack composition and order is defined in the "Layers" area.
  - *We set 2 layers: Al2O3 and HZO*
  - *We set thicknesses at 0.8nm and 7nm*
- Material properties of each layer can be loaded from *Material Library* by clicking the *book* icon ( )
  - *We here chose "Al2O3_default" and "HZO" respectively*
- (3) Device composition is updated

1. FTJ: Device creation





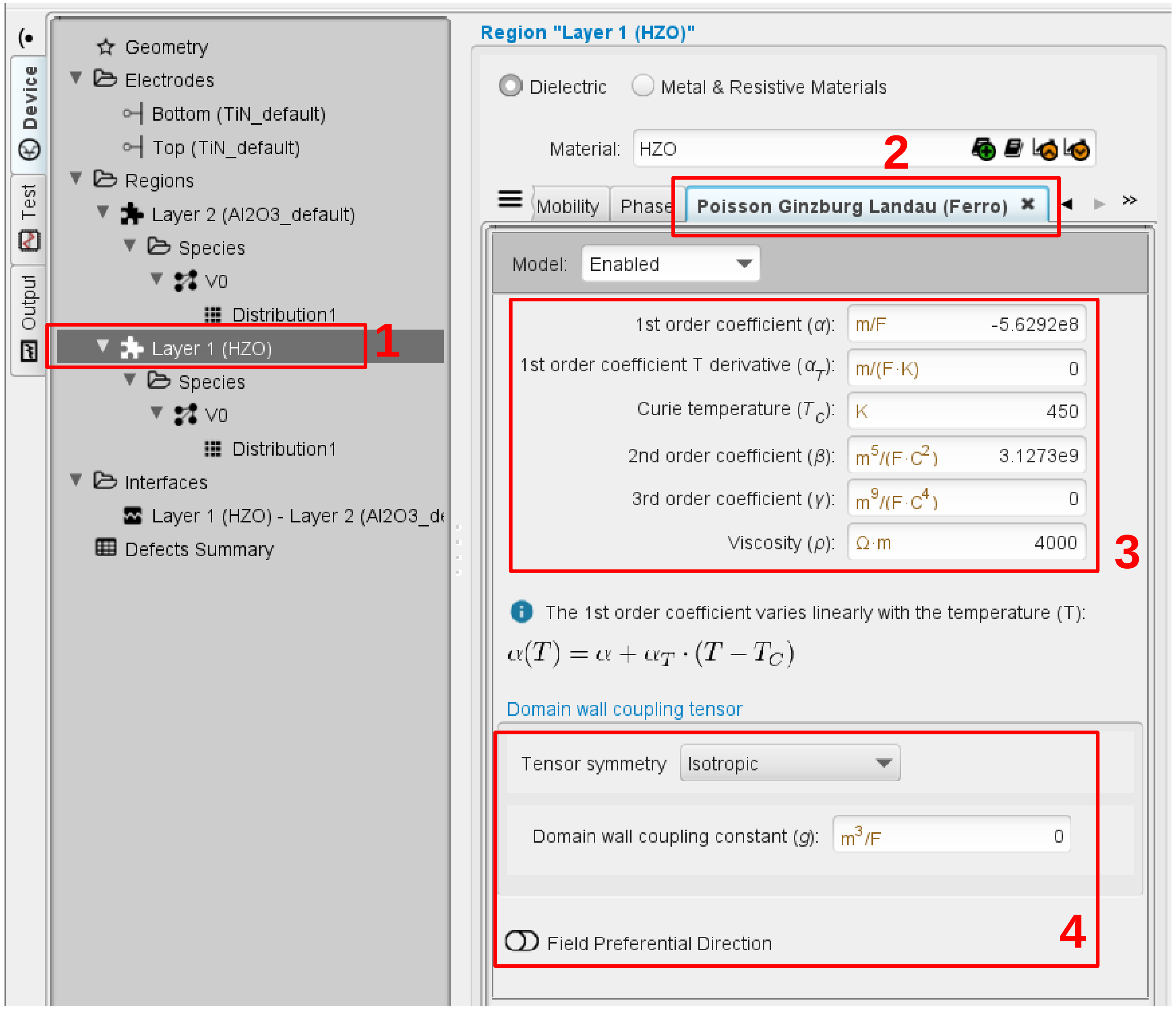
Electrode definition:

- (**4**) select each of the electrodes, (**5**) set the type and the (**6**) material
  - We set Electrodes to "Metals">"TiN_default"
- Set then the properties, depending on the type (e.g. for metallic: work functions; for semiconductor: doping)
  - We set Work Function to 4.75eV

Region Properties definition:

- (**7**) select each region and assign properties and enable/disable models
- It is possible to assign defect distributions with species properties and densities
  - We used default parameters for materials
  - We set Distribution density of V0 of Al_2O_3: 1e19 cm^{-3}
  - We set Distribution density of V0 of HZO: 5e19 cm^{-3}

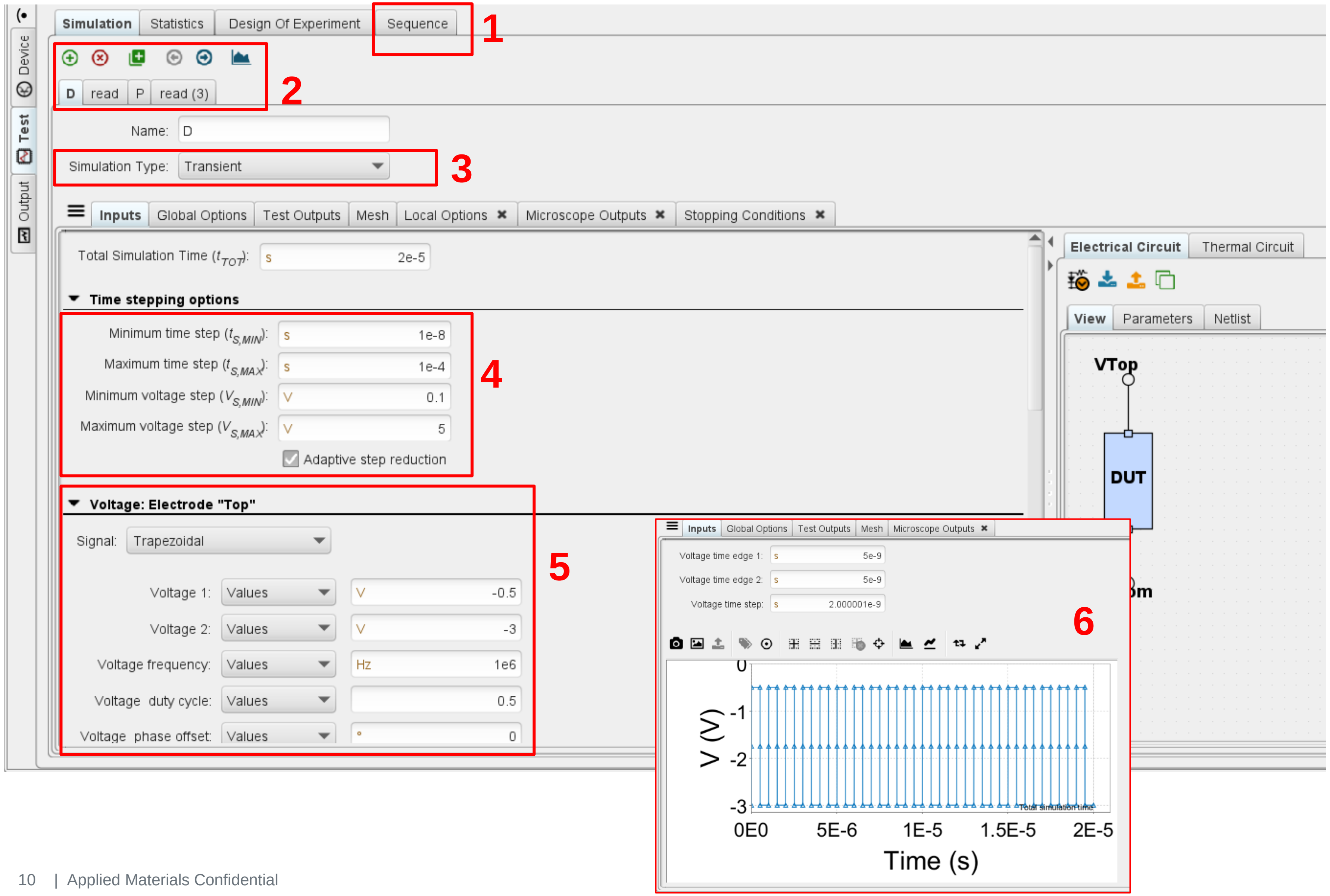
1. FTJ: Assign ferroelectric properties



1.3 PGL Parameters

- The last step in the creation of the device is the definition of the GL parameters.
- (**1**) select the *Layer 1 (“HZO”)* layer from the Device explorer tree.
- (**2**) select the *Poisson Ginzburg Landau (ferro)* tab (if not present pick the tab from ( ))
- (**3**) Set α, α_T, β, γ and ρ PGL parameters
  - We set parameters as in picture
- (**4**) Isotropy of domain coupling or preferential component of the field to be used for computation can be set.
- Similarly, the Preisach model can be enabled and set for ferroelectric description (just enable the respective tab, as explained above)

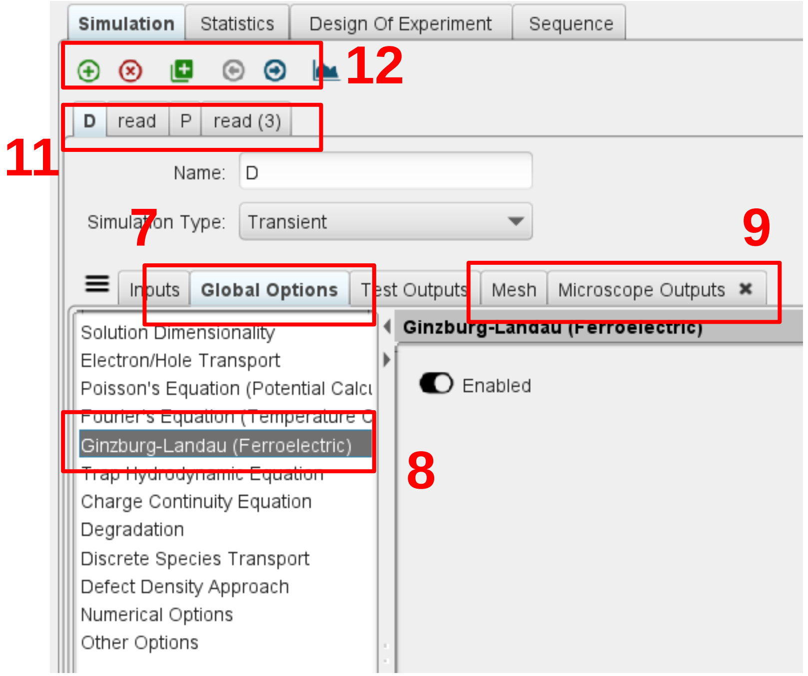
2. FTJ: Simulation setup

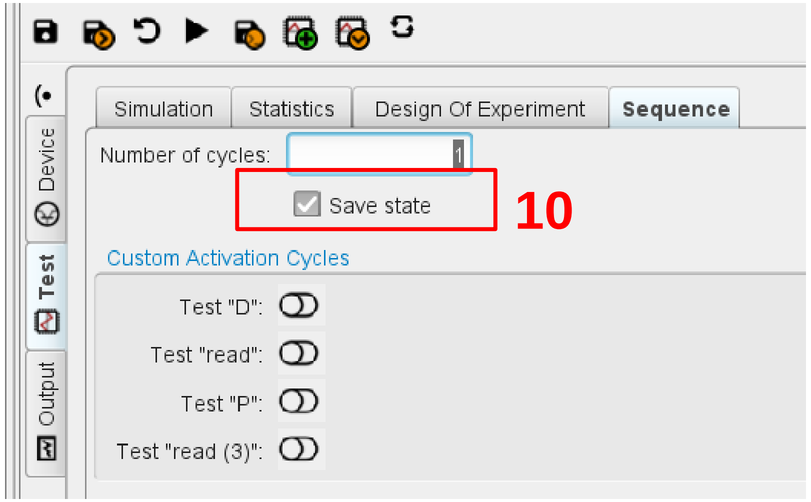


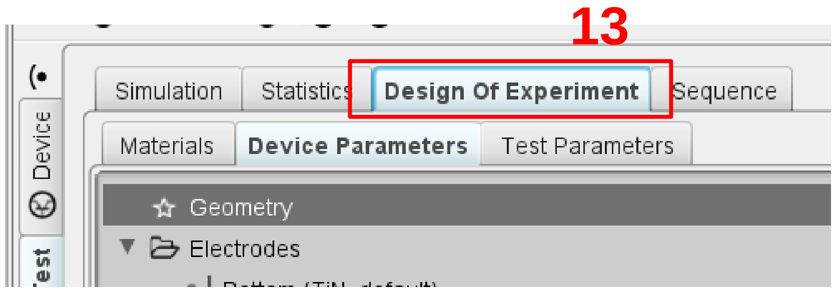
2.1 Simulation setup

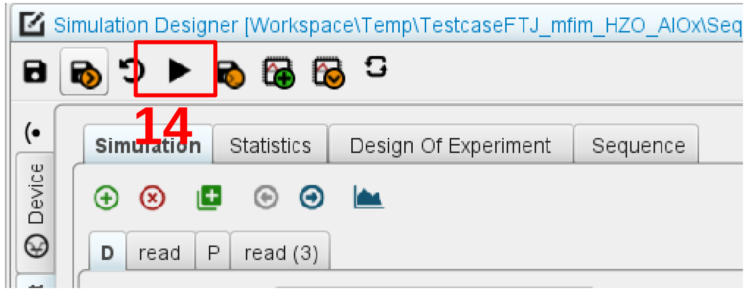
- **(2)** We defined here a *Sequence* of tests that will be run sequentially: *Depression>Read>Potentiation>Read.*
- *Sequence* is enabled in (**1**). State will be saved at the end of each sequence's step.
- **(3)** Test has to be a transient test for PGL model (it is time dependent)
- (**4**) set Stepping Options depending on the simulation
- (**5-6**) set input signal type for each of electrodes, with their properties and steps.
  - » We use "Trapezoidal" for Depression and Potentiation
  - » We use "Ramp" for Read tests

2. FTJ: Simulation setup









- **(7)** In Global Options all physical and numerical options can be set and models enabled
- **(8)** to enable GL computation in the stack, select *Ginzburg-Landau (Ferroelectric)* entry and enable the model with the switch.
- **(9)** Select the desired *Test outputs* and *Microscope outputs* (internal physical quantities) to be shown as results

Sequence setting:

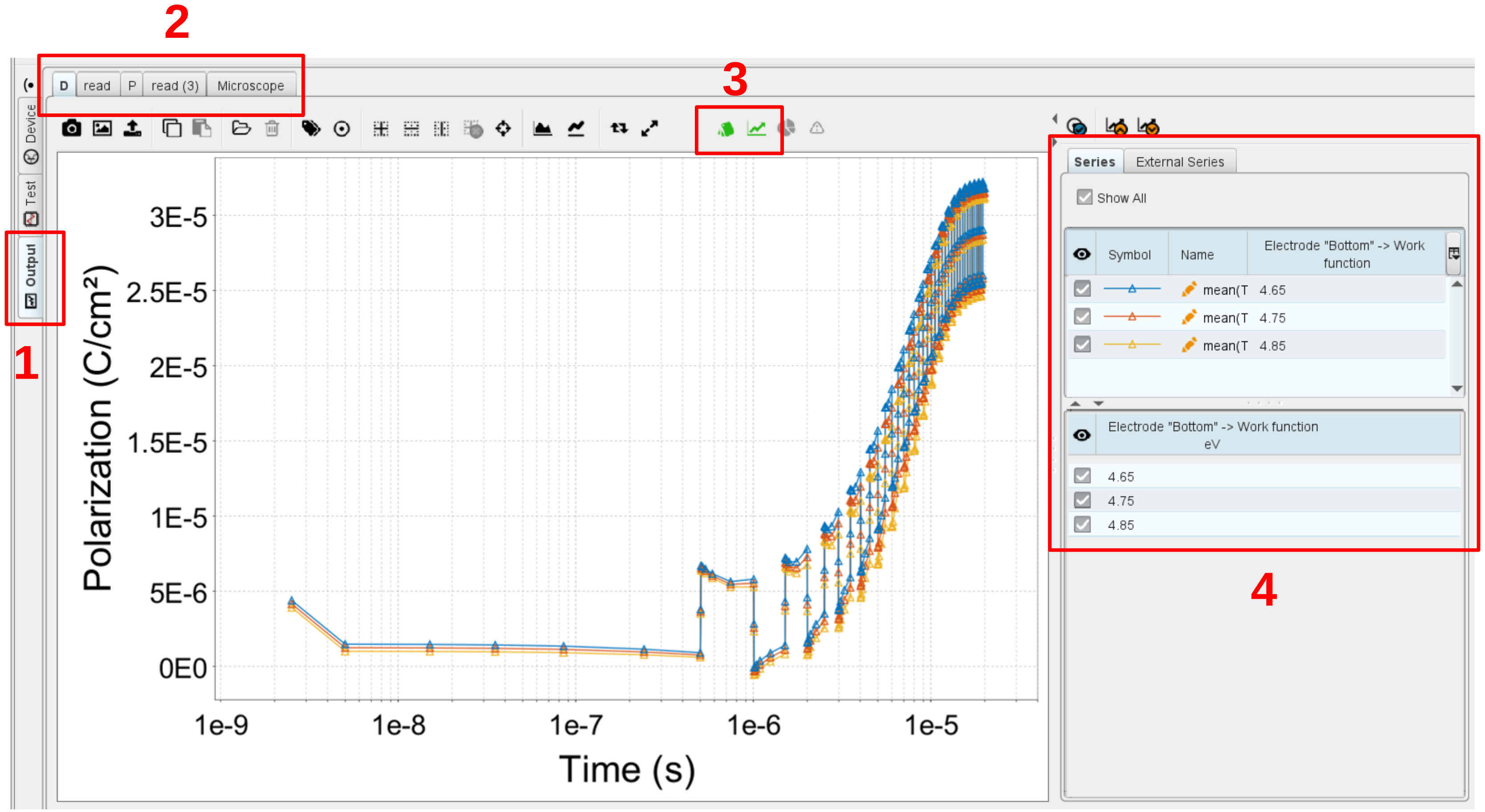
- **(10)** Enable "Save state" in the *Sequence* tab to allow correct concatenation of tests, as listed in (**11**).
- Sequence tests can be managed with buttons (**12**)

Design of experiments setting:

- **(13)** To enable DoE and set its entries

(14) Run Simulation

3. FTJ: Output analyses



3.1 Output management

- (**1**) Outputs are accessible through their tab at the end of the simulation
- (**2**) Test Output are produced for each of the sequence's tests + Microscope (providing internal physical outputs)
- (**3**) it is possible to choose x- and y-axes quantities (time, voltage, charges, etc.)
- (**4**) available list of curves