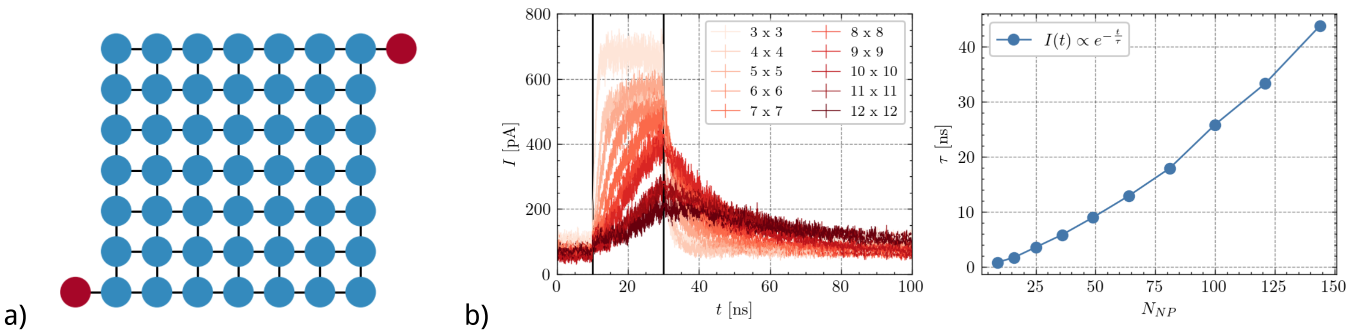
Step Input Response

Basics:

For a nanoparticle (NP) network of N_{NP} particles connected to two electrodes, we measure the electric current $I(t)$ response at the *output* electrode upon time varying voltages $U(t)$ at the *input* electrode. The voltage is changed within fixed time steps $$\Delta t = 10^{-10} \text{ s}$$ while the electric current is evaluated in those steps as the time average across the starting time t_i and the end time t_j of the corresponding step $$I(t) = \frac{e}{\Delta t} \cdot \sum_{t_0=t_i}^{t_j}(\Gamma_+(t_0) - \Gamma_-(t_0))\cdot t_0$$ with Γ_+ as the rate for a jump towards the output, Γ_- as the rate for a jump from the output, t_0 as the time passed for a single jump, and e as the elementary charge. If during the KMC procedure t_0 exceeds t_j we reverse the last event, won't consider the correponding rate difference and instead set $t_0 = t_i$ with t_i as the starting time of the next step.

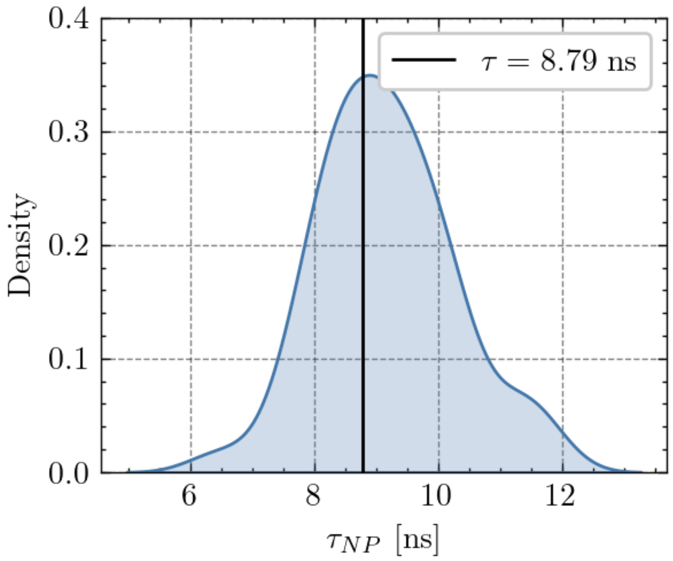
In each simulation we firstly equilibrate the system for $U(t=0)$ to receive the charge landscape $\vec{q}(t=0) := \vec{q}*{eq}$. The equilibrated landscape is stored and $N*{runs} = 500$ parallel simulations for the whole time scale are executed starting with $\vec{q}*{eq}$ as the initial landscape. We will then calculated the mean electric current in each time step t across all simulations $$\bar{I}(t) = \frac{1}{N*{runs}}\sum_{n=1}^{N_{runs}}I_n(t)$$ and the 95 % confidence interval for the mean estimate as $$\sigma_{\bar{I}}(t) = 1.96 \cdot \frac{\sigma_I}{\sqrt{N_{runs}}}$$ with electric current standard deviation σ_I.

Uniform Networks:



a) Network with 49 NPs and two electrodes marked red. b) Output electric current response for variable network sizes. The input electrode voltage signal is marked blue.

Firstly we analyse the output response in a uniform network of nanoparticles with equal nanoparticle sizes (electrostatic properties) and resistances (tunneling properties). The input voltage is switched based on $U \in {100 \text{ mV}, 200 \text{ mV}}$. The upper plots shows an example network and the responses for variable network sizes. We detect an exponential decline after the input voltage was reduced. When subtracting the y-axis offset of this decline, we are able to fit $$I(t) = I_0 \cdot e^{\frac{t}{\tau}} \Leftrightarrow \ln(I(t)) = ln(I_0) + \frac{t}{\tau}$$ and achieve the time relaxation time displayed above. We can use the same fitting process for the nanoparticle potentials:

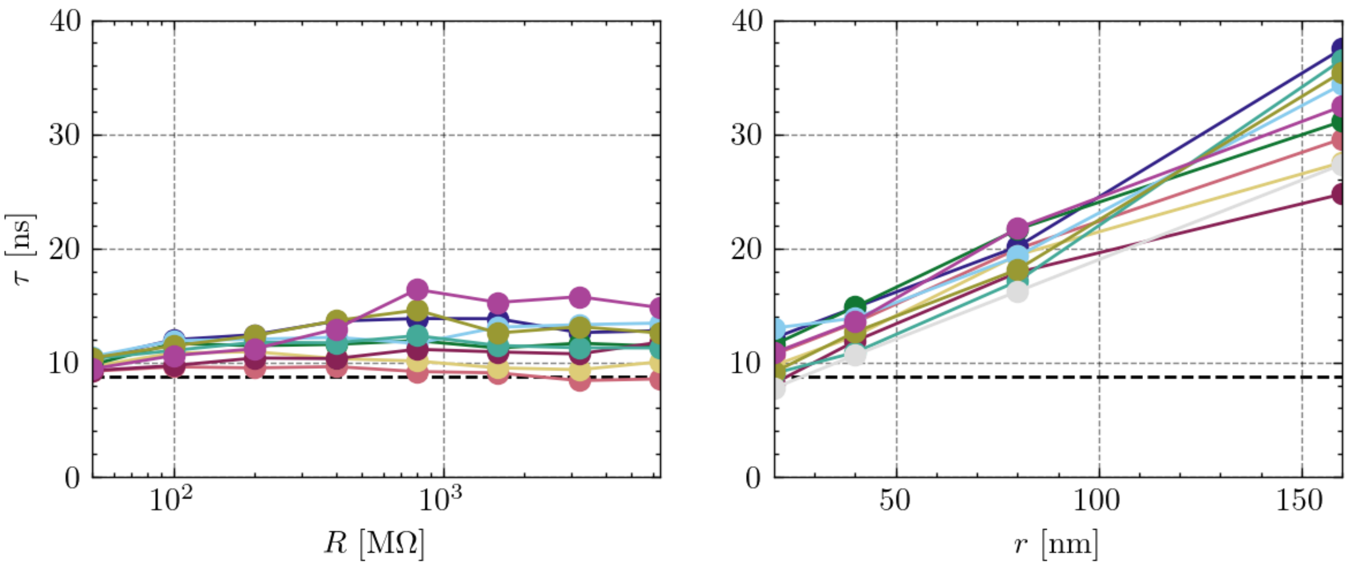


For a network of 49 NPs the distribution indicates variable relaxation times across the nanoparticles. Output relaxation time marked black.

Disordered Networks

We repeat the upper analysis for networks with disordered properties. There are three properties which can be coosen to be disordered:

Topology	Resistances	Nanoparticle Sizes
Network of $N_{NP} = 49$ NPs connected based on a *random regular graph* with node degree $N_j = 4$.	For a cubic shaped network of $N_{NP} = 49$ Nps all junction resistances are initially set at 25 MΩ. Next 9 NPs are choosen at random based on a given *seed*. Junctions connected to those NPs get a different resistance of R.	For a cubic shaped network of $N_{NP} = 49$ Nps all nanoparticle sizes are set at 10 nm. Next 9 NPs are choosen at random based on a given *seed*. Those NPs get a different radius of r.



Relaxation time for different distributions of disorder in terms of nanoparticle sizes and resistances. Black dashed line indicates uniform network.