Internship proposal: Ionic assemblies in subnanometric confinement

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As global access to water and energy supply is becoming an ever-more urging need, new technological solutions have been proposed based on nanofluidic membranes made of nanometric pores, carbon nanotubes, or atomically-thin graphene slits for water desalination or osmotic energy harvesting.

Very recently, the field has seen major advances as the two-dimensional confinement of water down to a single molecular layer was demonstrated experimentally in graphene slits. However, two-dimensional electrolytes are a virgin territory for theory: as confinement induces increased interactions and reduced dimensionality, their statistical properties wildly deviates from that of usual bulk electrolytes. In particular, very recent work in our group has shown that in experimentally-accessible ångströmetric confinement, ions should assemble into pairs, or even into "ionic strings" when an external electric field is applied (see Figure).

The dynamics of such ionic assemblies are still very poorly understood, and their shape, topology and size depend on the nature of the electrolyte. Interestingly, this entirely new phenomenology leads to memory effects in the system's dynamics which can be built on to replicate the functionalities of biological neutrons.

The goal of the internship would be to study the out-of-equilibrium dynamics of ionic assemblies, using both molecular dynamics simulations and analytical tools from statistical mechanics. Further work may include the study of bio-inspired "intelligent" ionic machines based on the unique properties of confined electrolytes.

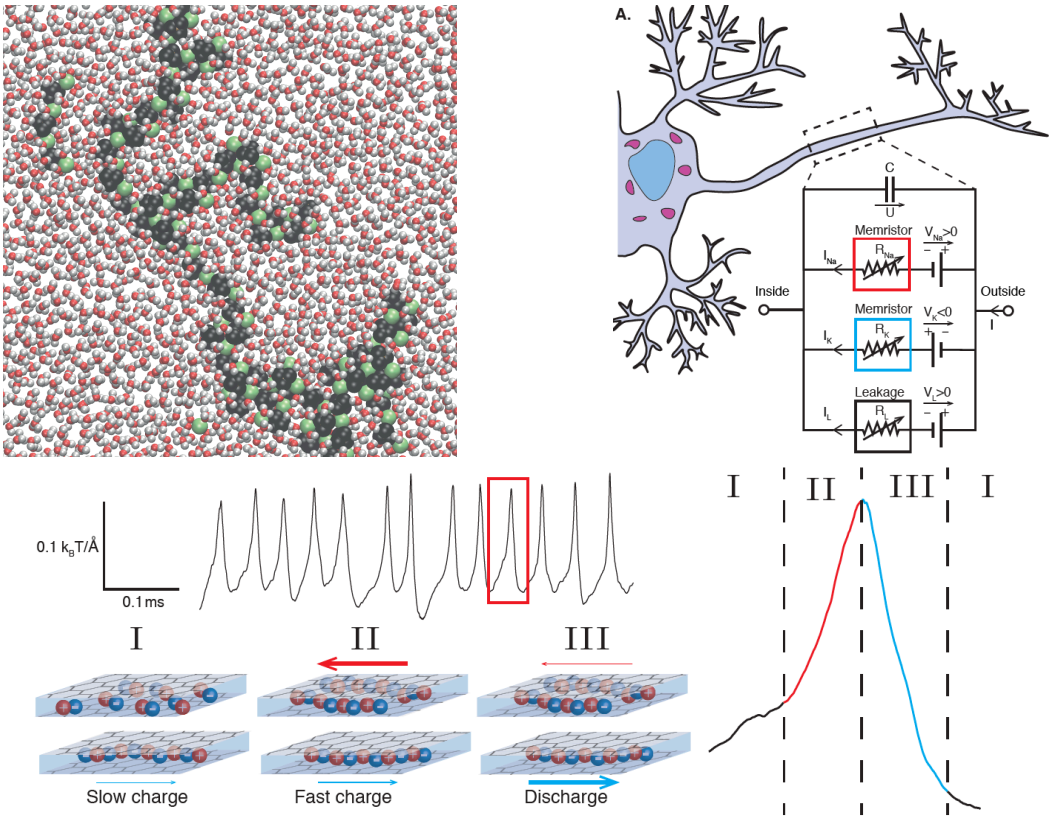

Figure: Ionic string formed by aqueous CaSO4 in nanometric confinement (top left). Prototype artificial neutron based on 2D confined electrolytes (top right and bottom).