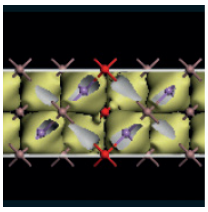

Session: Organic Semiconductor Devices/Soft Matter

(Invited) Towards the understanding of the mechanism of ions permeation through graphene-based membranes

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Permeation through nanometer pores is important in the design of materials for filtration and separation techniques and because of unusual fundamental behaviour arising at the molecular scale. Membranes comprising or incorporating graphene or graphene oxide (GO) offer remarkable potential for selective uptake and transport of molecular or ionic species. [1, 4] This high selectivity makes these membrane perfect candidates for membrane filtration technology. For a rational design of such nanomaterial the mechanism of permeation through the graphene layers need to be however fully understood and explained. Simulations can help in guiding the design of these extraordinary materials. In this talk we will present some recent results on GO-membrane and the challenges that molecular models face in simulating the real device.

[1] Nair *et al.*, *Science*, 2012, *335*, 442
[2] Joshi et al., *Science*, 2014, *343*, 6172
[3] Abraham et al., Nat. Nano, 2017, doi:10.1038/nnano.2017.21
[4] Williams et al., *J. Phys. Chem. Lett*, 2017, 8, 703

Simulation of tunneling based biosensor considering ion transport and electron tunneling

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Our group developed a reference electrode-free biosensor device having concentric electrode structure. (see Fig. 1.) An island electrode, hereafter called the drain, acts as a driving electrode, and an enclosing electrode, called the source, as a grounded electrode. Since the source electrode is bigger than the drain electrode, the electric potential of electrolyte is close to the source electrode as shown in Fig. 2., which shows the self-gating effect [1]. Recently, we extended the structure to detect matrix metalloproteinase9 (MMP-9), which is known as a biomarker of cancer cells. We immobilize the peptide substrate conjugated with methylene blue (MB) specific to MMP-9. Electron tunneling occurs between the MB and the drain electrode. As the MMP-9 cleaves the peptide, tunneling current between the MB states and drain electrode decreases [2]. We explain the influence of the ion transport on tunneling effect in this sensor using an in-house simulator. MODEL The simulation includes the three parts; Poisson equation, ion transport in the electrolyte system and the tunneling between the MB states and the electrode.