Soft Matter

ROYAL SOCIETY OF CHEMISTRY

Supplementary Information

Exploring the Potential of Ionic Bipolar Diodes for Chemical Neural Interfaces

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Figure S1. D⁺ concentration profiles around the AEM for reverse bias. The D⁺ concentration at the CEM-AEM interface (z = 0) decreases drastically for higher applied voltages.



Figure S2. The concentrations of mobile ions within the CEM channel in forward bias varies with AEM IEC. For higher IEC, more coions are injected into the CEM channel from the diode. This leads to higher conductivities and thus higher forward bias currents.



Figure S3. Diode current responses to a step in V_T from 1 V. The current stabilizes within 100 µs after an initial peak, probably caused by a discharging effect of the diode junction.



Figure S4. Na⁺ diffusion gradients within the AEM for different IEC (1.5 -> 0.15 M, blue -> yellow). The concentration of coins (Na⁺) in the AEM next to the electrolyte (to the right) is determined by the IEC of the AEM. Lower IECs give higher Na⁺ concentrations, thus a steeper diffusion gradient and higher reverse bias currents.



Figure S5. Device performance dependence on the IEC of the CEM loading channel. **a)** In reverse bias (VT = 1 V), higher CEM IEC gives lower D+ concentration at the outlet ($z = 2 \mu m$), i.e. reduces the leakage. **b)** In forward bias, higher CEM IEC gives higher D+ concentration at the outlet. This is caused by the higher D+ concentration in the CEM beneath the AEM. **c)** The diode current saturates at higher potentials for lower CEM IEC. **d)** The voltage over the CEM-AEM junction (V(z = 10 nm) – V(z = -10 nm)) is higher for higher CEM IEC, which explains why higher CEM IEC reduces the leakage. High leakage currents result in less current in the left part of the CEM channel, which causes the potential in the CEM at the diode to increase, thus lower junction voltage.





Figure S6. Electric potential at the outlet versus the bulk of the electrolyte for 100 nm and 200 nm thick AEMs of 1.5 M IEC. In reverse bias the voltage is approximately -2 mV and -1 mV for d = 100 nm and 200 nm, respectively. In forward bias the induced voltage depends on the applied V_T and reaches 23 mV for $V_T = -2$ V for the 200 nm AEM.

Figure S7. Effect of the transition zone between CEM and AEM layers. D⁺ concentration at $z = 2 \mu m$ for $V_T = 1 V$ for different widths of the transition zone between the CEM and AEM materials. The transition is implemented by a smoothed Heaviside function with a continuous second derivative without overshoot.



Figure S8. Meshing of the model. a) The mesh of the full model.b) The mesh from the top side when the electrolyte reservoir has been hidden. c) The mesh of the AEM in the diode. The two black areas are the densely meshed interfaces of the AEM.