UNIVERSITÄT DUISBURG ESSEN

Offen im Denken

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Dielectric effects on the ion flow near plain and polymer functionalized interfaces

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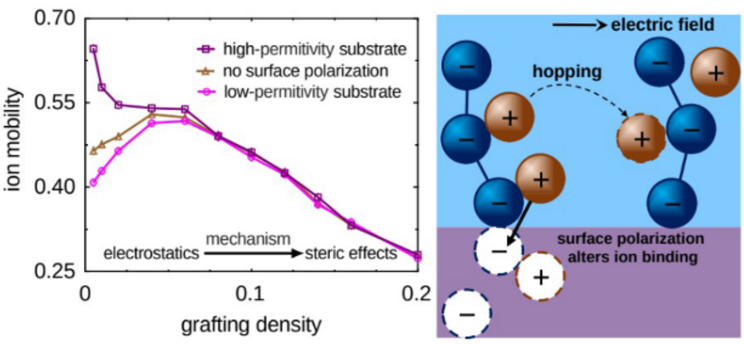
Fig. 1. Left: Ion conduction in PEBs is non monotonic as function of grafting density and affected by dielectric properties of the substrate. Right: schematic of the ion conduction mechanism and the surface polarization effect.



With the rise of nanofluidics, understanding and being able to control the movement of ions at the nanoscale is becoming more and more relevant. Indeed, ion mobility and ionic conductance in nanodevices are known to deviate from bulk behavior, a phenomenon often attributed to surface effects. Using coarse-grained molecular dynamics simulations, we have demonstrated that dielectric mismatch between the electrolyte and the surface can qualitatively alter ionic transport in a counterintuitive manner (in violation of Kohlrausch' law): Instead of following the polarization-induced modulation of the concentration profile, mobility is enhanced or reduced by changes in the ionic atmosphere near the interface and affected by a polarization force parallel to the surface. An analogous phenomenon exists in nanochannels functionalized with polyelectrolyte brushes—a construct used, e.g., for ion gating and current rectification in nanofluidic ionic circuits. Therein, surface polarization can drastically affect the ion conduction via altering the polymer-ion binding near the interface, even turning the non-monotonous dependency of ion mobility from polymer density to monotonous (see Fig. 1).