Water desalination and other processes involving separation and recovery of ionic species are energy-intensive, cost-intensive and generate waste. This issue poses a particular challenge from the perspective of future fresh water supply: 98% of water available in our planet is sea or brackish water, and it is estimated that two thirds of the world will be dealing with water scarcity by 2025. Electrosorption of ions onto nano-structured electrodes is a process that could potentially enable deionization technologies with lower energy and cost requirements and less waste than traditional technology. During electrosorption, ions are reversibly captured in the vicinity of charged electrodes with applied potentials lower than 2 volts. We suggest that one of the key elements in successfully designing electrosorption-based technologies lies in our ability to tailor the electrosorption process and electrodes to the specific physicochemical characteristics of the target ionic species.

A combination of electrochemistry experiments and molecular modeling results will be presented to discuss the effects of ion type, nano-confinement and applied potential on the electrosorption capacity for alkaline metal ions onto model electrodes. Titanium dioxide nanotubes were used as model electrodes because these structures present uniform cylindrical pores whose characteristics can be tailored during fabrication. The results demonstrate that electrosorption capacity is not strictly proportional to surface area and applied potential for the nanostructured electrodes used in this work in contradiction to classical electrosorption theory. The results also suggest that there are minima in terms of electrosorption capacity at intermediate pore sizes, where competitive energy and steric hindrance effects may take place. A key implication of the results to be presented is that nanoporous materials with tailored pore sizes may be used to improve the absolute electrosorption capacity of an electrode, and when coupled with voltage, it is possible to tailor ion selectivity to ion type.