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Ion Separation using a Y-Junction Carbon Nanotube JAE HYUN PARK, Beckman Institute for Advanced Science and Technology, UIUC, SUSAN SINNOTT, Department of Materials Science and Engineering, University of Florida , NARAYANA ALURU, Department of Mechanical and Industrial Engineering and Beckman Institute for Advanced Science and Technology, UIUC — Using molecular dynamics simulations, we show that a Y-junction carbon nanotube can be used to separate potassium and chloride ions from a KCl solution. The system consists of a KCl solution chamber connected to an (8,8) carbon nanotube, which acts as the stem. Two carbon nanotube branches of sizes (5,5) and (6,6) are connected to the (8,8) nanotube forming the Y-junction. Uncharged (5,5) and (6,6) carbon nanotubes show close to zero occupancy for transport of potassium and chloride ions. By functionalizing a (5,5) carbon nanotube with a negative charge, we show that we can selectively transport potassium ions. Similarly, by functionalizing a (6,6) carbon nanotube with a positive charge, we can selectively transport chloride ions. By performing molecular dynamics simulations on the entire system comprising the two branches, stem and the KCl solution chamber, we show that perfect ion separation is observed when (5,5) and (6,6) nanotubes are charged with $\sigma_{w,(5,5)} = -0.181$ C/m^2 and $\sigma_{w,(6,6)} = +0.143$ C/m^2, respectively, whereas for the system with $\sigma_{w,(5,5)} = -0.168$ C/m^2 and $\sigma_{w,(6,6)} = +0.131$ C/m^2 the separation is not perfect because of the formation of ion pairs. We discuss the formation and control of ion pairing, which is a common phenomenon in confined nanochannels.

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