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Asymmetric behavior in electrowetting of electrolyte solutions on graphene at the nanoscale: A molecular dynamics simulation FERESHTE TAHERIAN TABASI, Postdoctoral Research Fellow, NICO VAN DER VEGT, Professor of Physical chemistry at Technical University of Darmstadt — Using molecular dynamics simulations, electrowetting of aqueous solutions on graphene are studied. By doping the surface with the positive or negative charges, the counter-ions are adsorbed at the solid-liquid interface, and the co-ions are repelled from the interface, leading to the decrease of the solid-liquid surface tension and therefore the contact angle (known as electrowetting). Our simulation results show that at zero surface charge density, water molecules at the interface (located between the surface and first ionic layer) are mainly oriented parallel to the surface. However due to the smaller size of the hydrogen than the oxygen, there is a slight tendency of the water dipole moment to orient into the surface. On the charged surfaces, the orientation polarization of the interfacial water molecules are shown to be stronger on the negative surfaces than the positive ones. Such asymmetric orientation polarization of water leads to different screening of the graphene surface charge and therefore different contact angles of the solution on surfaces with opposite charges. Simulations results show more spreading of the liquid on the positively charged surfaces than the negative ones.

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