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Atomistic simulation study of charge inversion in silica nanochannels[1] CHRISTIAN D. LORENZ, ALEX TRAVESSET, Department of Physics and Astronomy, Iowa State University and Ames Laboratory — Recent experiments report charge inversion, i.e. interfacial charges attracting couterions in excess of their own nominal charge, in divalent ionic solutions near charged silicon oxide interfaces. We have conducted a series of atomistic molecular dynamics simulations in order to investigate the mechanism of charge inversion in these systems. We studied both $CaCl_2$ and $MgCl_2$ solutions near an amorphous silica substrate which had a charge density of $\sim 1/50\text{Å}^2$. Our simulation results give a detailed description of the structure of the ions and water near the silica interface. Finally, we show that our simulations are in remarkable agreement with the experimental results.

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