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Squeezout of a model ionic liquid under confinement and charging[1] ERIO TOSATTI, SISSA and ICTP, Trieste, Italy, ROSARIO CAPOZZA, SISSA, Trieste, Italy, ANDREA BENASSI, Empa, Duebendorf, Switzerland, ANDREA VANOSSI, CNR-IOM Democritos and SISSA, Trieste, Italy — Electrical charging of parallel plates confining a model ionic liquid down to nanoscale distances yields a variety of charge-induced changes in the structural features of the confined film, including even-odd switching of the structural layering, and important changes of planar ordering within layers. By means of molecular dynamics simulations, we explore this variety of phenomena in the simplest charged Lennard-Jones coarse-grained model including the effect a neutral tail attached to one of the model ions. Using open, grand-canonical-like conditions which allow the flow of ions in and out of the interplate gap, we simulate the liquid squeezout and obtain the distance dependent forces between the plates during their adiabatic approach under load. Effective free energy curves obtained by integration of these forces versus interplate distance show the local minima that correspond to layering, and predict the switching between one and another under squeezing and charging.

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