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**Charge Inversion by Electrostatic Complexation: Molecular Dynamics Simulations** JORDI FARAUDO, Universitat Autonoma de Barcelona, ALEX TRAVESSET, Iowa State University — Ions near interfaces play an important role in many biological and physico-chemical processes and exhibit a fascinating diverse range of phenomena. A relevant example is charge inversion, where interfacial charges attract counterions in excess of their own nominal charge, thus leading to an inversion of the sign of the interfacial charge. In this work, we argue that in the case of amphiphilic interfaces, charge inversion can be generated by *complexation*, that is, electrostatic complexes containing several counterions bound to amphiphilic molecules. The formation of these complexes require the presence at the interface of groups with conformational degrees of freedom with many electronegative atoms. We illustrate this mechanism by analyzing all atomic molecular dynamics simulations of a DMPA (Dimirystoil-Phosphatidic acid) phospholipid monolayer in contact with divalent counterions. The results are found to be in agreement with recent experimental results on Langmuir monolayers. We also discuss the implications for biological systems, as Phosphatidic acid is emerging as a key signaling phospholipid.

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