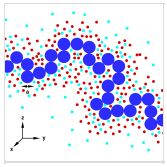

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Polyelectrolyte-chain-at-equilibrium

Mike Edwards[1]
[1]IPFDD

1 Works for me dx.doi.org/10.17504/protocols.io.bsmwnc7e

Mike J. Edwards
Tech. support phone: **+49 1746 125371** email: **edwards.ph@yahoo.com**

Mike Edwards

SUBMIT TO PLOS ONE

ABSTRACT

By means of the density functional theory framework (DFT) as well as the molecular dynamic simulations (MD), a polyelectrolyte chain (PE) in the good solvent conditions at thermal equilibrium is studied. The strength of the electrostatic interactions is varied by the Bjerrum length of the solvent. It turns out that average extension of a PE scales with the degree of polymerization, very much similar to a neutral polymer chain in good solvent. Remarkably, the difference between a PE and a neutral chain appears to be solely in the correlations among monomers which are stored in the Virial coefficients. Interestingly, upon increasing the Bjerrum length of solvent, the chain shrinks. This outcome is confirmed by the DFT framework as well as the MD simulations. The significance of this study is that it strongly criticizes the idea (already mentioned in T. Kreer, *Soft Matter*, **12**, 3479 (2016)) that the PEs behave similar to a neutral ideal chain. This study could be useful in our understanding of biopolymers.

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KEYWORDS

Polyelectrolyte, Density functional theory framework (DFT), Debye-Hueckel potential, Molecular dynamic simulations (MD)

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