

Abstract Submitted
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Model for evaluating patterned charge regulation contribution to electrostatic interactions between proteins¹ DAWN HOLLENBECK, K. MICHAEL MARTINI, ANDREAS LANGNER, DAVID ROSS, ANTHONY HARKIN, EDWARD NELSON, GEORGE THURSTON, Rochester Institute of Technology — We study the pattern-specific work of charging for two spherical model proteins in close proximity in ionic solution, using a grand-canonical partition function together with a coarse-grained, linear Debye-Huckel model to calculate the needed work of charging for each possible proton occupancy configuration. We seek to delineate a parameter-space phase diagram to characterize the circumstances under which patterned charge regulation, attractions due to heterogeneous protein charging patterns, and screened net protein charge could individually dominate the electrostatic portion of the interaction between model particles. Within the model, we place titratable residues in accordance with the tertiary protein structure, as is done in the case of a single protein within the Tanford-Kirkwood protein electrostatics model. We use Monte-Carlo simulation and analytical work to evaluate how the local statistics of the charging patterns on each protein respond to close proximity and relative orientation of neighboring proteins.

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