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Electrostatics in a Crowded World: Bridging Theory and Cellular Reality in Macromolecular Interactions

Electrostatic interactions are fundamental drivers of macromolecular structure, recognition, and function. The pioneering work of Sharp and Honig established how these forces can be rigorously described through continuum electrostatics and molecular dynamics, offering predictive frameworks to quantify the delicate balance between charged residues and the surrounding solvent. Complementing this theoretical foundation, Mittal' s contributions underscore the cellular context—where macromolecules exist in an environment of extreme crowding, confinement, and heterogeneity. Such conditions modulate electrostatic interactions in ways that can enhance stability, alter conformational landscapes, or disrupt associations altogether. Together, these perspectives reveal that electrostatics cannot be divorced from the physicochemical reality of the cell. While theoretical models provide mechanistic precision, the principle of macromolecular crowding captures the emergent complexity of life at the molecular scale. An integrated view highlights that the behavior of biological macromolecules is governed not only by long-range electrostatic forces, but also by the crowded, fluctuating milieu that defines living matter.

Key words: Electrostatic interactions, Macromolecular crowding, Continuum electrostatics, Molecular dynamics, Biomolecular interactions, Protein stability

Author: Dr M, Manjula (Department of Physics and Electronics, Jain University)

Presenter: Dr M, Manjula (Department of Physics and Electronics, Jain University)

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