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Deciphering adhesion forces in mussel-inspired peptides

Nature offers a rich repertoire of adhesive materials derived from plants, animals, and microorganisms, promising transformative applications in under water construction and biomedicine. Despite their potential, translating these natural materials into practical applications remains challenging due to a limited understanding of their underlying adhesion mechanisms. To bridge this knowledge gap and accelerate the development of bioinspired adhesives, in this talk I present a molecularthermodynamic model for predicting the adhesion forces of mussel-inspired peptides under various solution conditions. The coarse-grained model accounts for the sequence characteristics of amino-acid residues based on their electrical charge, excluded molecular volume, and other non-electrostatic interactions including the surface binding capability. Its numerical performance was validated with experimental data from surface force measurements for three mussel-inspired peptides. We find that the optimal adhesion to the surface reflects a delicate balance between electrostatic attraction and hydrogen binding. By incorporating a genetic algorithm to explore the peptide sequence space, we demonstrate that the adhesion strength of mussel-derived peptides can be improved by nearly one third.