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Strong adsorption of random heteropolymers on protein surfaces
TRUNG NGUYEN, Northwestern University, BAOFU QIAO, Argonne National Laboratory, BRIAN PANGANIBAN, CHRISTOPHER DELRE, TING XU, University of California, Berkeley, MONICA OLVERA DE LA CRUZ, Northwestern University — Rational design of copolymers for stablizing proteins' functionalities in unfavorable solvents and delivering nanoparticles through organic membranes demands a thorough understanding of how the proteins and colloids are encapsulated by a given type of copolymers. Random heteropolymers (RHPs), a special family of copolymers with random segment order, have long been recognized as a promising coating materials due to their biomimetic behaviors while allowing for much flexibility in the synthesis procedure. Of practical importance is the ability to predict the conditions under which a given family of random heteropolymers would provide optimal encapsulation. Here we investigate the key factors that govern the adsorption of RHPs on the surface of a model protein. Using coarse-grained molecular simulation we identify the conditions under which the model protein is fully covered by the polymers. We have examined the nanometer-level details of the adsorbed polymer chains and found a clear connection between the surface coverage and adsorption strength, solvent selectivity and the volume fraction of adsorbing monomers. The results in this work set the stage for further investigation on engineering biomimetic RHPs for stabilizing and delivering functional proteins across multiple media.

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