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Theory and Computational Design of Protein Materials

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Protein design opens routes to arrive at novel molecules, materials and nanostructures. Recent theoretical methods can identify the properties of amino acid sequences consistent with desired structures and functions. Such methods leverage concepts from statistical mechanics and address the structural complexity of proteins and their many possible amino acid sequences. Computationally designed protein-based systems have been experimentally realized to encapsulate nonbiological cofactors and assemble into predetermined crystalline structures.