De novo Protein Generation for Enhanced Efficiency in Biohybrid Solar Cells

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Solar energy's vast abundance makes it a leading candidate for Earth's growing sustainable energy demands. However, traditional photovoltaic solar cells face many limitations such as high space requirements and a maximum possible efficiency as governed by the Shockley-Queisser limit. Biohybrid solar cells offer a promising alternative by leveraging natural light-harvesting mechanisms found in photosynthesis to maximize the efficiency of light absorption in solar cells. Despite their potential, current biohybrid approaches suffer from protein instability and inefficiency outside their native plant environments, rapidly denaturing under harsher conditions. This project addresses these challenges by designing novel proteins optimized for use in biohybrid solar cells. The proteins are engineered for enhanced light absorption, electron transfer efficiency, thermostability, and binding affinity with chromophores and semiconductor materials. To achieve this, we developed a hybrid-process by judiciously combining artificial intelligence and machine learning, genetic algorithms, and mathematical abstractions and analysis. The first step uses a deep learning transformer to generate proteins. Secondly, a validator evaluates protein properties based on mathematical algorithms and provides feedback to enhance the generator's output. In the third step, an optimizer refines the proteins using a genetic algorithm to improve performance. Lastly, non-dominated sorting is used to select the best protein candidates that excel across all performance metrics. This method of protein abstraction using autotrophic principles and photovoltaics aims to generate highly efficient and stable proteins for biohybrid solar cells, offering a breakthrough in renewable energy.

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