SolarEye: Novel Solar Energy Harvesting Retinal Molecule Derivative and Rhodopsin Inspired Protein Scaffold Biomaterial Designed by Utilizing a Large-Language-Model and Computational Tools

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Current organic photovoltaics (OPV) have narrow light absorbance, inefficient electron transport, and low energy output. This project aims to solve these efficiency issues by designing an organic biomaterial derived from the retinal molecule and rhodopsin protein complex. To create this material, a customized Chemical Large-Language-Model was designed to derive the retinal molecule structure for widened light absorption and efficient electron transport properties. Computational tools were utilized to design a rhodopsin inspired protein scaffold (RIPS) to support the retinal derivative structure in electron transport. Time Dependent Density Functional Theory calculations found the derivative had a wide light absorption bandwidth of 472 nanometers (nm) (from 450nm-950nm), with 3.66% more wavelength coverage than current OPVs. The strongest absorption peak was found at 919.23nm and the second strongest at 512nm, indicating high absorbance at both the infrared and visible spectrum. Electrostatic potential maps and frontier molecular orbital visualization revealed that the molecule's electrons donate and redistribute from photon absorption, showing strong evidence of electron donation and low recombination. Electrostatic potential maps illustrated that RIPS acted as an "electron piston" to help donate electrons of the retinal derivative. Finally, the Power Conversion Efficiency revealed a value of 7.37%, which is 1.37% higher than current OPVs, indicating higher energy output. Overall, this novel biomaterial is an improved organic photovoltaic through wider light range absorption, more efficient electron transport systems, and higher energy output.

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