

CONSTRUCTING A DE NOVO CHARGE SEPARATING TRIAD.

Paul Molinaro, Ronald Koder

Department of Physics, City College of New York, New York, NY

Light activate charge separation can provide high energy electrons for a variety of chemical processes. Our objective is to create a four helical bundle that will act as the scaffold for a charge separation triad, which will produce long-lasting charge-separated states with high efficiency. Our previous designs required careful biochemistry to assemble and never produced detectable charge separation. Thankfully, the availability of user-friendly software packages has greatly minimized the time investment needed to produce new designs and screen them in silico. Our approach utilizes both physical tools (protCAD and openMM) and machine learning techniques (Alphafold and proteinMPNN) to design and screen charge separation scaffolds. The design workflow is presented in this poster.

