

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

How to harvest solar energy with the photosynthetic reaction center. ALEXANDER BALAEFF, JUSTIN REYES, University of Central Florida — Photosynthetic reaction center (PRC) is a protein complex that performs a key step in photosynthesis: the electron-hole separation driven by photon absorption. The PRC has a great promise for applications in solar energy harvesting and photosensing. Such applications, however, are hampered by the difficulty in extracting the photogenerated electric charge from the PRC. To that end, it was proposed to attach the PRC to a molecular wire through which the charge could be collected. In order to find the attachment point for the wire that would maximize the rate of charge outflow from the PRC, we performed a computational study of the PRC from the *R. viridis* bacterium. An ensemble of PRC structures generated by a molecular dynamics simulation was used to calculate the rate of charge transport from the site of initial charge separation to several trial sites on the protein surface. The Pathways model was used to calculate the charge transfer rate in each step of the network of heme co-factors through which the charge transport was presumed to proceed. A simple kinetic model was then used to determine the overall rate of the multistep charge transport. The calculations revealed several candidate sites for the molecular wire attachment, recommended for experimental verification.

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Date submitted: 06 Nov 2015

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