Nano Letters 2015 vol.15 N3, pages 1722-1729

## Fast delocalization leads to robust long-range excitonic transfer in a large quantum chlorosome model

Sawaya N., Huh J., Fujita T., Saikin S., Aspuru-Guzik A. Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

## Abstract

© 2015 American Chemical Society. Chlorosomes are efficient light-harvesting antennas containing up to hundreds of thousands of bacteriochlorophyll molecules. With massively parallel computer hardware, we use a nonperturbative stochastic Schrödinger equation, while including an atomistically derived spectral density, to study excitonic energy transfer in a realistically sized chlorosome model. We find that fast short-range delocalization leads to robust long-range transfer due to the antennae's concentric-roll structure. Additionally, we discover anomalous behavior arising from different initial conditions, and outline general considerations for simulating excitonic systems on the nanometer to micrometer scale.

http://dx.doi.org/10.1021/nl504399d

## Keywords

Chlorosome, exciton, graphics processing unit, green sulfur bacteria, photosynthesis, spectral density