Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Theoretical Studies on Excitation Energy Fluctuations of Pigments in a Light-Harvesting Complex MASAHIRO HIGASHI, Univ of the Ryukyus, SHINJI SAITO, Insititute for Molecular Science — Excitation energy fluctuations of pigments in light-harvesting complexes play an important role in the excitation energy transfer dynamics. It is considered that protein environment controls the excitation energy fluctuation to maximize the efficiency of excitation energy transfer. However, the detailed mechanism is still unknown. The high computational cost of reliable electronic structure calculations for excited states prevents us from carrying out a large number of sampling needed to evaluate the excitation energy fluctuations. To overcome this difficulty, we develop a new method called molecular mechanics with Shepard interpolation corrections (MMSIC), which enable us to generate potential energy surfaces for pigments in light-harvesting complexes efficiently. We illustrate the new method by application to bacteriochlorophyll *a* pigments in the Fenna-Matthews-Olson complex. The MMSIC calculations are more than a million times faster than the direct electronic structure calculations, and the calculated results are in good agreement with the experimental results.

Masahiro Higashi
Univ of the Ryukyus

Date submitted: 09 Nov 2013 Electronic form version 1.4