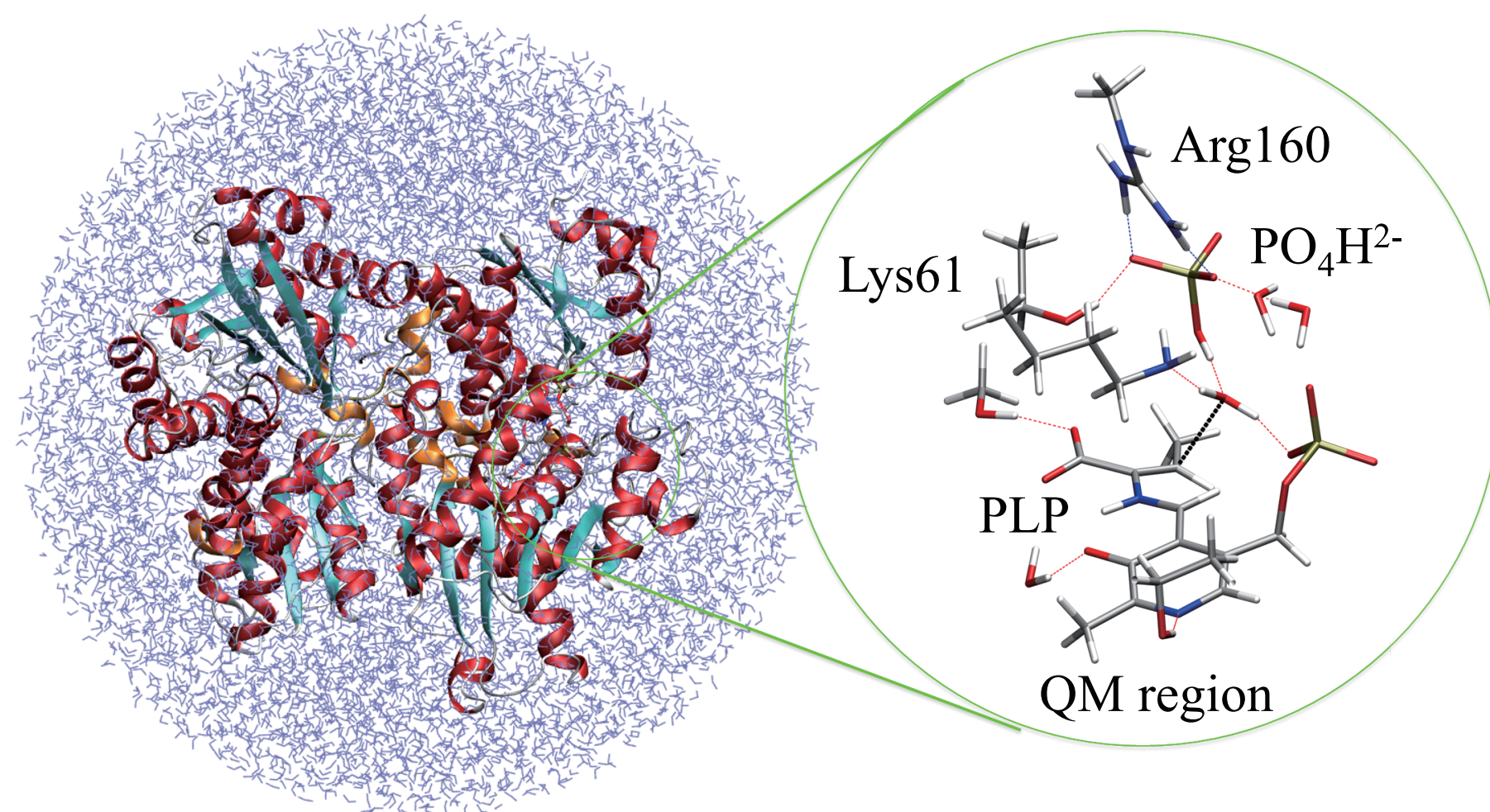


Biological Sciences on HA-PACS/COMA

QM/MM studies on catalytic reactions in enzymes

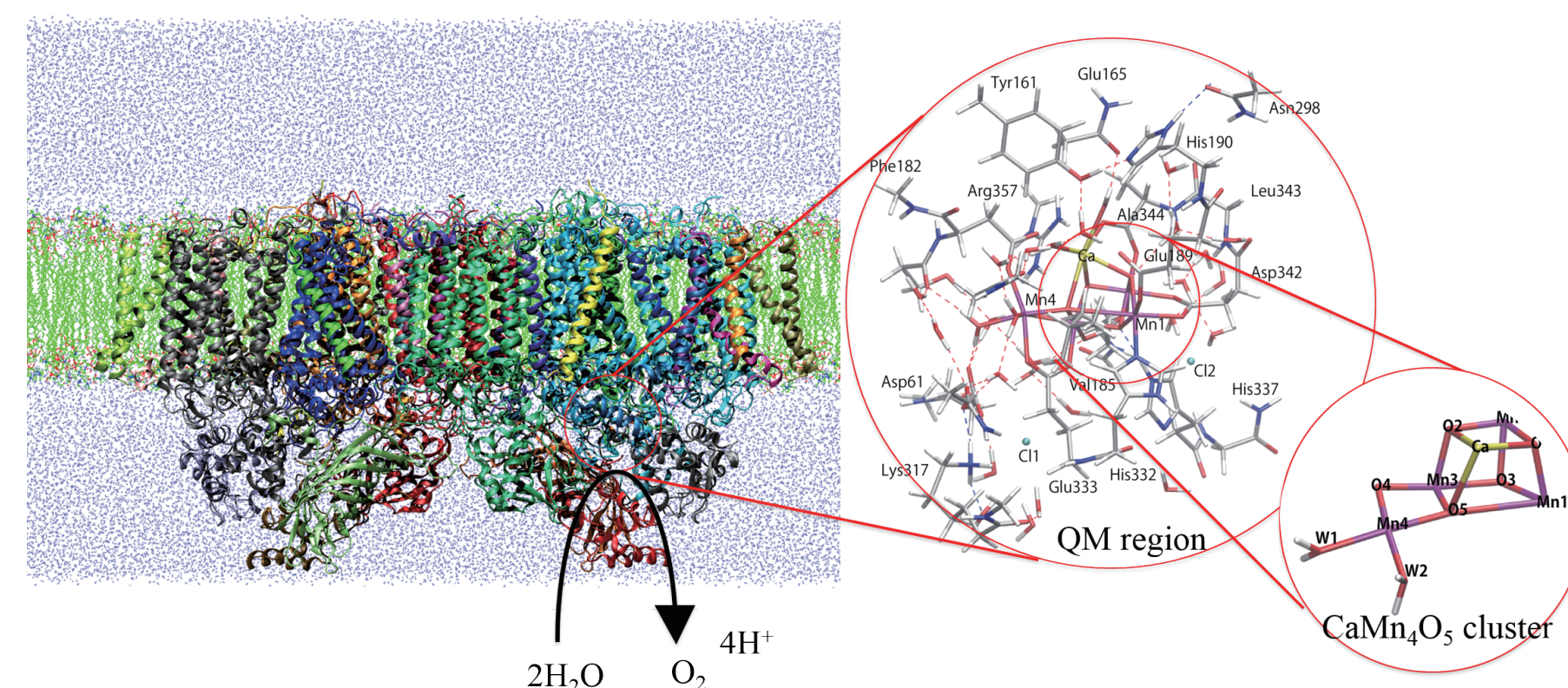
Threonine Synthase (ThrS)



Threonine synthase (TS) catalyzes the last step of L-Thr biosynthesis and its reaction is the most complex among the PLP enzymes. To elucidate the detailed mechanism, we performed comparative QM/MM calculations with an exhaustive search for the reaction pathways in the reaction-specificity-determining-process. Satisfactory agreements with the experimental data were obtained. Contrary to the earlier proposal, the base that abstracts a proton from the attacking water was the Lys61 amino group rather than the phosphate ion. We also determined that phosphate ion forms a stable hydrogen bond with the PLP-Thr moiety, which is critical for the reaction specificity. Additionally, a new mechanism was proposed for the transaldimination process [1].

[1] M. Shoji et al., *J. Am. Chem. Soc.* **136**(12), 4525 (2014).

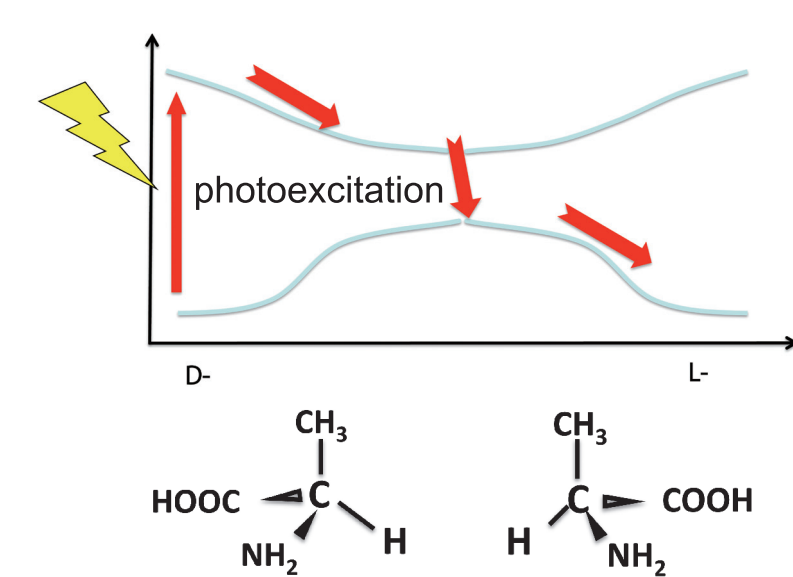
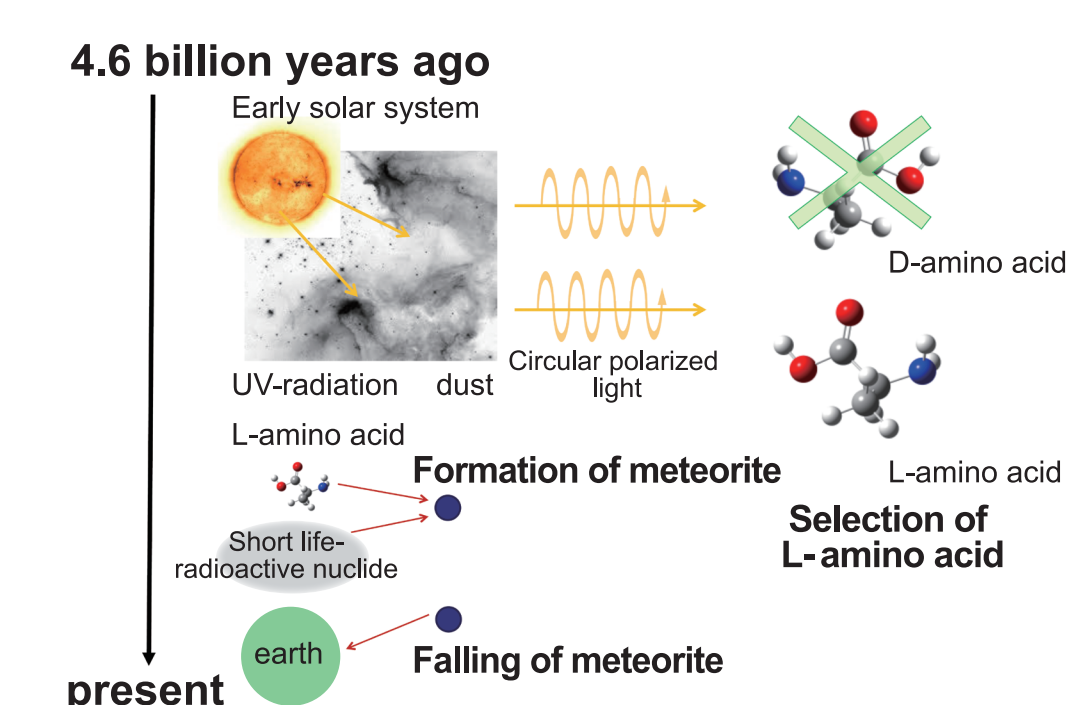
Oxygen-Evolving Complex in Photosystem II (OEC-PSII)



Oxygen-evolving complex (OEC) is a key reaction center in photosystem II (PSII) which catalyzes " $2\text{H}_2\text{O} \rightarrow 4\text{H}^+ + \text{O}_2$ " reaction through five redox states (S_i , $i = 0-4$). J.-R. Shen, N. Kamiya and co-workers have determined a high-resolution PSII x-ray structure and it was found that OEC is involved in many hydrogen-bonds (H-bonds) with water molecules and neighboring amino acid residues, however, it is still matter of debates for the reaction mechanisms. We investigated the OEC electronic structures by using a high level QM/MM approach. We adopted a large QM region including second coordination amino acids and waters (Total 380 atoms, 3000 basis functions) and investigated possible protonation states and electronic structures. OEC core structures and calculated quantum ground state are in good agreements with experimental results.

[2] M. Shoji et al., *Catal. Sci. Technol.*, **3**, 1831 (2013). [3] M. Shoji et al., *Mol. Phys.* 2014 in press.

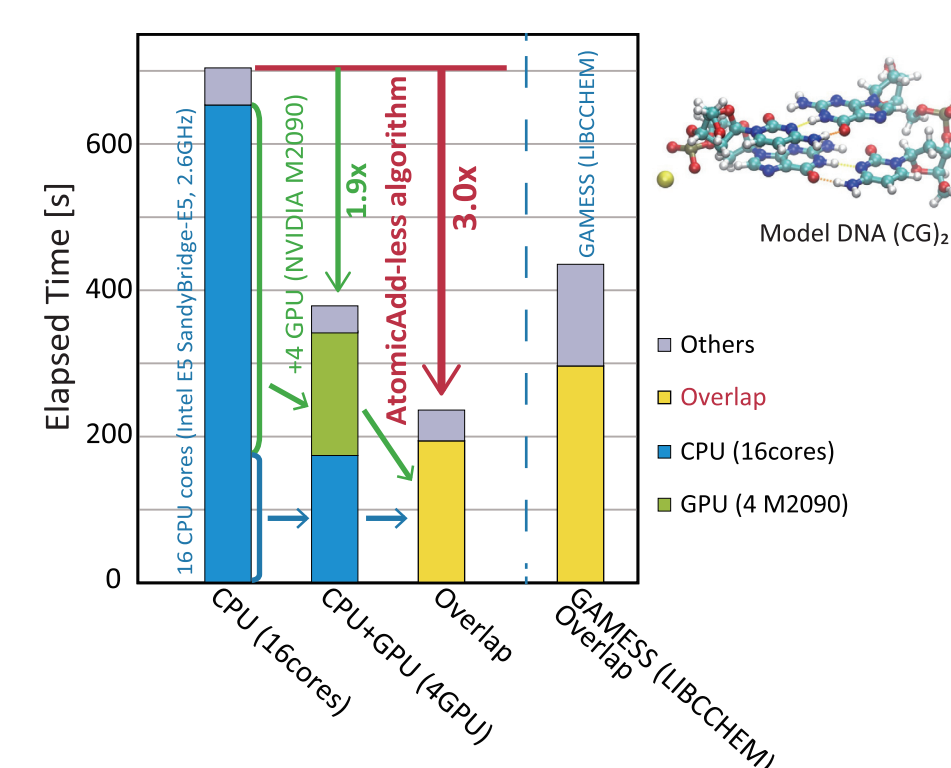
Astrobiology Chirality Formation of Amino Acids in the Early Solar System



The naturally-occurring amino acids in terrestrial life are all the levorotatory (L-) form, none of the D-form. The origin for its selectivity still remains a big mystery. One of the possible scenarios is that the chiral induction of amino acids is formed on meteorites in the early solar systems [4]. In order to validate the hypothesis, we have investigated the mechanisms of photo-induced chirality formation by using the TDDFT method. Circular dichroism and UV-absorbance spectrum were calculated for amino acids and plausible chiral induction mechanisms were discussed.

[4] J. R. Cronin et. al., *Science* 275, 951 (1997); M. H. Engel et. al., *Nature* 389, 265 (1997).

GPU Accelerated Molecular Orbital Calculation



GPU accelerated Fock matrix preparation of a Hartree-Fock (HF) calculation routine, which is a basic and common process in various *ab initio* molecular orbital (MO) calculations, in the OpenFMO program [5] has been implemented. With our atomicAdd-less algorithm [6], total elapsed time was remarkably reduced. Figure shows timing results for a HF/6-31G(d) calculation of 126 atomic molecule (1,282 AO) performed by an HA-PACS base cluster node, which consists 16 CPU cores (Intel E5 Sandy Bridge-EP, 2.6GHz) and four GPU cards (NVIDIA M2090). Here, Fock matrix preparation tasks are assigned to CPU or GPU depending on GPU speedup ratio of corresponding integral type, and are performed with overlapping calculation.

[5] <http://www.openfmo.org/OpenFMO/>. [6] H. Umeda, et al., *IPJS Transactions on Advanced Computing Systems*, 6,4, 26-37 (2013).