

庄司光男 (公募 A 班)

会議発表

1. 庄司光男、磯部寛、重田育照、中嶋隆人、山口兆, “光化学系 II 酸素発生中心における Ca イオンの役割についての QM/MM 解析”, 第 99 回日本化学会春季年会, (日本, 2019/03/17)
2. Mitsuo Shoji, “Water Insertion Reactions of the Oxygen-Evolving Complex of Photosystem II Revealed by QM/MM”, Theoretical Chemistry Symposium 2019 (TCS2019), (Pilani, Rajasthan, India, 2019/2/14) [invited]
3. Mitsuo Shoji, “A new approach for searching reaction pathways applicable to quantum mechanical calculations”, CCS-EPCC Joint Workshop, (Edinburgh, UK, 2018/12/4) [invited]
4. 庄司光男、村川武志、重田育照、岡島俊英, “銅含有アミン酸化酵素におけるセミキノンラジカル生成機構についての理論的解明”, 第 32 回分子シミュレーション討論会, (茨城県つくば市, 日本, 2018/11/29)
5. M.Shoji, H.Isobe, Y.Shigeta, T.Nakajima, K.Yamaguchi, “Water insertion reactions in the oxygen-evolving complex of photosystem II revealed by QM/MM calculations”, ICPAC Langkawi 2018, (Langkawi Island, Malaysia, 2018/10/31) [invited]
6. M.Shoji, H.Isobe, Y.Shigeta, T.Nakajima, K.Yamaguchi, “QM/MM study on the O₂ formation and O₂ release mechanism in the oxygen-evolving complex of photosystem II”, the 56th Annual Meeting of The BioPhysical Society of Japan, (Okayama, Japan, 2018/09/16)
7. M.Shoji, H.Isobe, Y.Shigeta, T.Nakajima, K.Yamaguchi, “QM/MM study on the S state transitions of the oxygen-evolving complex in photosystem II”, the 43rd International Conference on Coordination Chemistry (ICCC2018), (Sendai, Miyagi, Japan, 2018/08/03) [invited]
8. 庄司光男, “分子構造および反応機構探索アルゴリズムの新展開”, 第 18 回日本蛋白質科学会年会, (新潟県新潟市, 日本, 2018/06/26)
9. M.Shoji, M.Kayanuma, Y.Shigeta, “A new algorithm searching stable molecular structures and reaction pathways by introducing repulsive interactions among walkers”, ICQC 2018, (Menton, France, 2018/06/20)
10. M.Shoji, M.Kayanuma, H.Kitoh-Nishioka, Y.Shigeta, “A new approach for searching stable molecular structures by introducing repulsive interactions among walkers”, 7thJCS, (Prague, Czech Republic, 2018/5/21-24)
11. 庄司光男、常盤恭樹、山崎笙太郎、栢沼愛、重田育照, “分子構造探索および反応経路探索のための新手法(GLAS 法)の提唱”, 第 21 回理論化学討論会, (愛知県岡崎市, 日本, 2018/05/16)