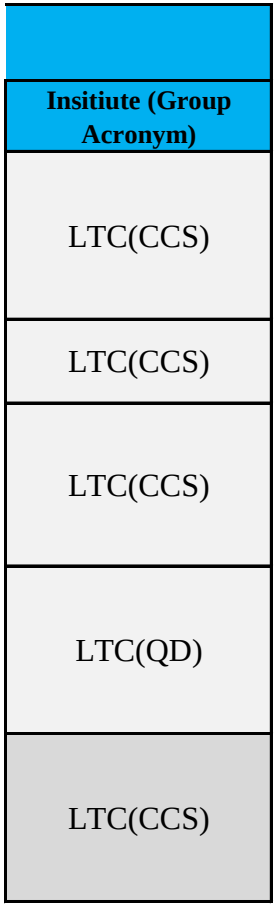
Institute/Department	Acronym	Group Leaders	Web Page
Laboratory of Theoretical Chemistry, Department of Molecular Engineering	CCS	Hirofumi Sato	www.riron.moleng.kyoto-u.ac.jp
Laboratory of Theoretical Chemistry, Department of Molecular Engineering	QD	Nguyen Thanh Phuc	https://researchmap.jp/thanh_phuc

METHODOLODOGY

General keyword	Details in topic	Researchers involved	Insitiute (Group Acronym)
Methodology for condensed chemical systems	Development of molecular statistical mechanics for liquids and solution phase	Hirofumi Sato	LTC(CCS)
	Hybrid mehtods of quantum chemistry and statistical mechanics		
	Kinetics and quantum chemistry of self-assembly process		
	Analysis of electronic structures of molecules		
Molecular quantum dynamics, open quantum systems, molecular polariton, light-matter interaction, condensed-matter physics	Studying quantum dynamics of condensed-phase molecular systems	Nguyen Thanh Phuc	LTC(QD)
	Studying quantum dynamics of light-matter coupled systems		

Electrochemistry	Developing approaches that hybridize electronic structure theories and molecular dynamics simulations to study electrode-electrolyte interfaces	Hiroshi Nakano	LTC(CCS)

APPLICATIONS			
Systems	**Property**	**Methods**	**Researchers involved**
Solution phase and liquids	chemical reactions, photoprocess, free energy, distribution functions, correlation functions	RISM, 3D-RISM, RISM-SCF-SEDD, 3D-RISM-SCF / Development of new equations and methods	Hirofumi Sato
Self assembly systems	stability, kinetics of the assembly	quantum effective hamiltonian / master equation	Hirofumi Sato
Organic molecules	intepretation of electronic structure	second quantisation operator	Hirofumi Sato
Condensed-phase molecular systems strongly coupled to an optical cavity	Effects of molecular polariton formation on molecular quantum dynamics	Analytical and numerical methods	Nguyen Thanh Phuc
Electrochemical systems, electrode-electrolyte interfaces	Electrochemical reactions, capacities, optical response of electrochemical interfaces	hybrid methods combining electronic structure theroies and molecular dynamics simulations	Hiroshi Nakano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