# 新学術領域研究「水を主役とした ATP エネルギー変換」

## 前期(2008-2010)研究成果報告会

August 9-11, Osaka, Japan

Grant-in-Aid for Scientific Research on Innovative Area:

Hydration and ATP Energy

Ministry of Education, Culture, Sports, Science and Technology (MEXT)

Place: Hotel Osaka Garden Palace, 大阪府淀川区西宮原 1-3-35 TEL 06-6396-6211

使用言語 Language: 日本語もしくは英語 Japanese or English

Break 5 min

August 9 13:00-13:10

14:30 - 15:30

### Program

Opening Address ー領域の目標とこれまでの進展ー

	Purpose of this Program and the Progress			
	Makoto Suzuki	(Project Leader, Tohoku Univ.)		
13:10 – 14:25				
Extended views of hydration states of ions and ATP-related molecules				
	Chaired by N. Matubaya	si		
15	Nobuyuki Morimoto	(Tohoku Univ.)		
	Hydration properties of o	ligonucleic acid analyzed by microwave		
	dielectric spectroscopy			
15	Takuya Takahashi	(Ritsumeikan Univ.)		
	Assessment of dynamic properties of water around several solute			
	molecules with MD simulation			
15	Akifumi Ikehata	(NARO, Japan)		
	A novel interpretation of	near infrared spectra for detection of		
	volumetric change around hydrophobic groups			
15	•	(Japan Atomic Energy Agency)		
	Coupling of water dynamics and internal dynamics of actin detected			
	by neutron scattering			
15	Nobuo Niimura (Ibara	•		
	Hydration network structure in protein-ligand interface determined			
	by neutron diffraction.			

Thermodynamic views of ATP hydrolysis (Experimental approach)

	Chaired by T. Takahashi			
15	Yoshihiro Sambongi (Hiroshima Univ.)			
	Effects of salt on ATPase activity of halophilic archaeon <i>Haloarcula Japonica</i>			
15	Ryo Kanzaki (Kagoshima Univ.)			
	Thermodynamic study on ionization of nucleobases in micellar			
15	solution and ionic liquid Michie Vernanche (Kryschy Hritz)			
15	Michio Yamanaka (Kyushu Univ.) Partial molar volume study of ATP hydrolysis on bovine serum			
	albumin surface			
15	Masayoshi Nishiyama (Kyoto Univ.)			
	Visualization and manipulation of intermolecular interaction by high-pressure microscopy			
15:90 16:50				
15:30 – 16:50 Poster	r Session			
1 0,500.	. 2000-101-			
16:50– 18:35				
Nanos	structure and dynamics of ATP-driven proteins Chaired by Y. Sambongi			
15	Nobuhiro Morone (Kyoto Univ.)			
	Cellular structure-function analysis of ATP-related membrane protein			
15	Takayuki Ariga (Tokyo Univ.)			
1.5	Force generation mechanism of kinesin motor			
15	Hiroaki Yokota (Kyoto Univ.) Single-molecule ATPase imaging of a DNA helicase			
Theoretical approach for the ATP hydrolysis reaction				
	Chaired by M. Kinoshita			
15	Takeshi Yamamoto (Kyoto Univ.)			
	Ab initio study on the energetics of phosphate hydrolysis in water and			
15	organic solvents Hideaki Takahashi (Tohoku Univ.)			
10	Computation of the solvation free energies by the QM/MM-ER			
	approach: simplification of the method and its applications			
30	Minoru Sakurai (Tokyo Inst. Tech.)			
	Structural and dynamics changes of ABC transporters induced by ATP binding and its hydrolysis			
	ATT blitting and its flytholysis			
August 10				
9:00 - 10:30				
	nduced structural change of proteins			
	Chaired by R. Akiyama			
15	Hiroaki Kato (Kyoto Univ.)			
	Transmission mechanism of ATP-induced conformational changes in			
15	ABC transporter Masahiro Ishiura (Nagoya Univ.)			
10	ATPase activity of the cyanobacterial clock protein KaiC			
15	Taro Uyeda (AIST)			
	Uni-directional cooperative conformational changes of actin filaments:			
	possible implications in force generation by myosin			

30	Mitsunori Takano (Waseda Univ.) Atomic-level observation of ATP-induced allosteric responses of myosin motor domain by MD
10:15 – 11:45 Poster	Session
12:45 – 13:00 ATP-in-	Lunch duced structural change of proteins (continued)
15	Chaired by M. Sakurai Daron Standley (Osaka Univ.) Flipping the switch on an electrostatic gatekeeper controlling nucleotide specificity in succinyl-CoA synthetase
13:00 - 15:00	nacioonae specificity in succinyr correspinite asc
	and cosolvent effects on the ATP systems
15	Shun-ichi Kidokoro (Nagaoka Univ. Tech) Overall- and elementary-reaction enthalpies of ATP hydrolysis evaluated by isothermal titration calorimetry
15	Hideyuki Komatsu (Kyushu Inst. Tech.) Solvent mixtures mimicking a nucleotide-binding feature of ATPase
15	Kuniyuki Hatori (Yamagata Univ.) Effects of urea and guanidine hydrochloride on actomyosin functions
15	Mitsuhiro Iwaki (Osaka Univ.) Actomyosin motility revealed by single-molecule Measurements
15	Ryo Akiyama (Kyushu Univ.)  Effective Interaction between like-charged macromolecules in an electrolyte solution and cytomotive filaments
Ticc	Break 10 min.
Effects	of ATP-driven proteins on the medium Chaired by M. Iwaki
15	Takuo Yasunaga (Kyushu Inst. Tech.)
30	Approach to direct observation of environmental electrostatic fields around actin-myosin filaments in water by electron microscopy Makoto Suzuki (Tohoku University)
	Opposing hydration properties of charged and hydrophobic groups and cosolvent effects on protein hydration and functions
15:10 – 16:30	Poster Session
16:30 – 18:30	
	g force and energy balance in F1-motor
	Chaired by M. Kinoshita
30	Eiro Muneyuki (Chuo Univ.)
30	Energetic balance in single molecule F1-motor Mitsunori Ikeguchi (Yokohama City Univ.)
	Theoretical study on rotational mechanism of F1 molecular motor and asymmetric structures

### Theoretical progress on ATP-driven protein systems

Theoretical progress of the arrived process systems				
	Chaired by M. Suzuki	(Tohoku Univ.)		
30	Masahiro Kinoshita	(Kyoto Univ.)		
	Roles of water and ATP hydrolysis in functioning of ATP-driven			
	proteins			
30	Nobuyuki Matubayasi	(Kyoto Univ.)		
	All-atom analysis of solvent effect on ATP and related systems			
18:45 - 20:30	Banquet			
August 11				
0.00 0.00	C DE CONTRA	2000 2010		
8:00-9:00	Summary Meeting of FY			
	Makoto Suzuki (Tohoku	Univ.)		

評価委員 中村春木(大阪大学蛋白質研究所) 永山國昭(生理学研究所) 柳田敏雄(大阪大学)

### 顧問

児玉孝雄 (大阪大学)

学術調査官 門田 功(岡山大学) 曽和義幸(法政大学)

### 総括研究班

鈴木 誠 (東北大学) 木下 正弘 (京都大学) 松林 伸幸 (京都大学) 櫻井 実 (東京工業大学)

#### 領域代表:

鈴木 誠 東北大学大学院工学研究科 材料システム工学専攻教授 〒980-8579 宮城県仙台市青葉区荒巻字青葉 6-6-02 022-795-7303 (phone/fax)