

Symposium on Hydration and ATP Energy 2013

Hotel Iwanuma-ya, Akiu, Sendai, Japan
http://www.iwanumaya.co.jp/e_web/
March 6 (Wed)– 8(Fri), 2013.

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The Ministry of Education, Culture, Sports, Science and Technology (MEXT)
<http://www.material.tohoku.ac.jp/atpwater/index.htm>

Organizing and Program Committee

Makoto Suzuki (Project Leader, Tohoku University) : Chair
Nobuyuki Matubayasi (Kyoto University)
Masahiro Kinoshita (Kyoto University)
Minoru Sakurai (Tokyo Institute of Technology)

March 6

13:00-13:10

Opening address

Makoto Suzuki (Tohoku University)

Session 1 “Hydration effects on molecular motors”

chaired by Yoshihiro Sambongi (Hiroshima University)

13:10-13:40

Hiroaki Yokota (Kyoto University)

L1 : Single-molecule imaging of ATPase reactions catalyzed by a DNA helicase

13:40-14:10

Toshiki Yagi (Tokyo University)

L2 : Effects of salts or cosolvents on flagellar axoneme structure and motility

14:10-14:40

Mitsuhiro Iwaki (Osaka University)

L3 : Dynamics and energetics of actomyosin motor in the presence of osmolyte

14:40-15:10

Masayoshi Nishiyama (Kyoto University)

L4 : Microscopic analysis of the motility of single bio-nanomachines at high-pressure

15:10-15:30

Break

- 15:30-17:00 **Poster preview**
 chaired by Nobuyuki Matubayasi(Kyoto University)
- 17:00-18:00 **Poster session I**
- 19:00-21:00 **Dinner time**
- 21:00 – 23:00 **Group meeting** (A01, A02, A03)

March 7

Session 2 “Structure and dynamics of ATP-driven proteins”

chaired by Eiro Muneyuki(Chuo University)

- 9:00-9:30 Takeyuki Wakabayashi (Teikyo University)
L5 : Activation of myosin ATPase by mutant actins
- 9:30-10:00 Takeshi Murata(Chiba University)
L6 : Rotation mechanism of *Enterococcus hirae* V1-ATPase based on asymmetric crystal structures
- 10:00-10:30 Yoshiro Sohma (Keio University)
L7 : ATP hydrolysis-driven gating mechanism of an ABC transporter CFTR channel
- 10:30-11:00 Minoru Sakurai (Tokyo Institute of Technology)
L8 : Roles of ATP and water in the functional mechanism of ABC transporters. Computational approaches based on MD simulation and theories of solution
- Special lecture** *chaired by Makoto Suzuki(Tohoku University)*
- 11:00-12:00 Werner Kunz (Regensburg University)
 “Hydration phenomena around ions, osmolytes, hydrotropes and charged protein or surfactant headgroups”
- 12:00-13:00 **Lunch Break**
- 13:00-15:00 **Poster session II**

Session 3 “Energetics of ATP hydrolysis”

chaired by Takuya Takahashi(Ritsumeikan University)

- 15:00-15:30 Norio Yoshida (Kyushu University)
L9 : Free Energy Analysis of ATP hydrolysis based on the statistical mechanics and quantum mechanics theory
- 15:30-16:00 Hideaki Takahashi(Tohoku University)
L10 : Free energy analysis of the hydrolysis of the prototype molecule for ATP

16:00-16:30	Hideyuki Komatsu (Kyushu Institute of Technology) L11 : Thermodynamics of partitioning of ATP, ADP and Pi between water and organic solvent
16:30-17:00	Yoshihiro Sambongi (Hiroshima University) L12 : Salt dependency of inorganic pyrophosphatase activity in an extremely halophilic archaeon <i>Haloarcula japonica</i>
17:00-18:00	Poster session III
19:00-21:00	Banquet
21:00-23:00	Summary meeting (A01, A02, A03 groups)

March 8

Session 4 “Hydration structure and dynamics from ions to proteins”

chaied by Minoru Sakurai(Tokyo Inst. Technology)

9:00-9:30	Ryo Akiyama(Kyushu University) L13 : Hydration dynamics and dielectric relaxation of water around an ion
9:30-10:00	Koji Yoshida(Fukuoka University) L14 : A study on hydration structure of F-actin by X-ray scattering
10:00-10:30	Nobuo Niimura((Ibaraki University) L15 : The hydration structure and dynamics of proteins determined by neutron protein crystallography
10:30-11:00	Satoru Fujiwara (JAEA) L16 : Hydration water around F-actin studied by neutron scattering
11:00-11:45	Session 5 “Summary of the project” Nobuyuki Matubayasi(Kyoto University) Makoto Suzuki (Tohoku University)
11:45-12:00	Concluding Remarks and Information from MEXT Yasuteru Shigeta(MEXT, Osaka University) Makoto Suzuki(Tohoku University)
12:00	Closing