Computational Approaches for the Study of Chemical and Biological Systems

Joint Spanish-Japanese Symposium. 23rd November, 2015

Centro de Investigaciones Biológicas, CIB-CSIC. Madrid, Spain

Organizers: Sonsoles Martín-Santamaría and Shigeyoshi Sakaki

The symposium will bring together researchers from both countries showing different approaches from the computational chemistry to address the study of chemical and biological systems.

Attendance to the lectures will be **free of charge**, although **we kindly ask all attendees to register** (contact Lucía Pérez Regidor, lucia.perez.regidor@cib.csic.es). Deadline: 18th November 2015.

Venue: http://www.cib.csic.es/en/como_llegar.php

Session I

9:00 hrs. Opening.

9:15 hrs. Plenary lecture. **Keiji Morokuma.** *Fukui Institute for Fundamental Chemistry. Kyoto Universit. Kyoto, Japan.*
Computational studies of chemical reactions of complex molecular systems.

10:00 hrs. Plenary lecture. **Federico Gago.** *University of Alcalá. Alcalá de Henares, Spain.*
***In silico* pharmacology: from molecular simulations to structure-activity relationships and structure-based drug design**.

10:45-11:15 hrs. Coffee break.

Session II

11:15 hrs. **Masataka Nagaoka.** *Nagoya Univeristy. Nagoya, Japan.*
"Allosteric" regulation through dynamical intermolecular interactions between proteins and small molecules/cations.

11:40 hrs. **Sonsoles Martín-Santamaría.** *Center for Biological Research, CIB-CSIC. Madrid, Spain.*
Molecular modeling in molecular recognition. Pattern recognitions receptors.

12:05 hrs. **Shigeyoshi Sakaki.** *Fukui Institute for Fundamental Chemistry. Kyoto University. Kyoto, Japan.*
Catalysis by transition metal complex. Use of unusual valence state and Lewis acid.

12:30 hrs. **Laura Masgrau.** *University Autonomous of Barcelona. Barcelona, Spain.*
Computational modeling of enzymatic mechanisms.

12:55-14:45- Free time for lunch.

Session III

14:45 hrs. **Jyun-ya Hasegawa.** *Catalysis Research Center. Hokaido University. Sapporo, Japan.*
Excited states and molecular interactions in photofunctional proteins.

15:10 hrs. **Miho Hatanaka.** *Kinki University. Osaka, Japan.*
Theoretical study of lanthanide luminescence for thermo- and biosensors.

15:35 hrs. **Luis M. Frutos**. *University of Alcalá. Alcalá de Henares, Spain.*
Photoactive proteins and photoactive molecular devices.

16:00-16:15 hrs. Short break.

Session IV

16:15 hrs. **Masahiro Ehara.** *Institute for Molecular Science. Okazaki, Japan.*
High throughput computations of solvent effects using PCM SAC-CI approach.

16:40 hrs. **Ugo Bastolla.** *Center for Molecular Biology, CBM-CSIC. Madrid, Spain*.
Computing protein dynamics from protein structure with elastic network models.

17:05-17:30 hrs. Closing remarks.
Shigeyoshi Sakaki & Sonsoles Martín-Santamaría.
Institutes and activities around theoretical chemistry in Japan and Spain. A meeting point.

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