International Conference on Computational Science and Technology 2014

(ICCST2014)

15-16 May 2014, Institute of Physics Polish Academy of Sciences, Warsaw, Poland

Programme

Thursday, 15 May 2014

8:30-9:40 Registration

9:40-10:00 Opening Section

SECTION I Computational Chemistry and Material Science

Chairperson: Duc Nguyen-Manh

10:00-10:30 Minh Tho Nguyen, University of Leuven, Belgium

Computational Quantum Chemistry at Leuven

10:30-11:00 Truong Ba Tai, University of Leuven, Belgium

Disk-aromaticity and its application for polycyclic compounds

11:00-11:30 *Coffee Break*

Chairperson: Minh Tho Nguyen

11:30-12:00 S. Roszak, Wrocław University of Technology, Poland

Quantum chemistry – the efficient first step for designing materials of desired properties

12:00-12:30 Thuat T Trinh, Norwegian University of Science and Technology, Trondheim, Norway

Prediction of Chemical Potential and Activity Coefficient of Graphite Surface from Molecular Dynamics Simulation

12:30-13:00 Duc Nguyen-Manh, Culham Centre for Fusion Energy, UK

Integrated modeling approach for nuclear fusion, material science and engineering

13:00-14:30 **Lunch and Poster Section**

Chairperson: S. Roszak

14:30-15:00 Vu Thi Ngan, Qui Nhon University, Vietnam

Interesting properties found in doped silicon clusters

15:00-15:30 R. Buczko, Institute of Physics PAS, Warsaw, Poland

Surface states of topological crystalline insulators

15:30-16:00 *Coffee Break*

16:00-16:30 Alesander Gabovich, Institute of Physics NASU, Kiev, Ukraine

Stationary Josephson current between d-wave superconductors with charge density waves: angular dependences and violations of the corresponding-states relationship

16:30-17:00 Vinh Hung Tran, Institute of Low Temperature and Structure Research PAS, Wroclaw, Poland

Electronic Structure of Selected Strongly Correlated Electron Systems

19:00-22:00 CONFERENCE BANQUET

Friday 16 May 2014

SECTION II COPUTATIONAL BIOPHYSICS AND MEDICINE

Chairperson: Mai Suan Li

9:30-10:00 Andrzej Koliński, University of Warsaw, Poland

CABS - coarse grained modeling of protein structure assembly, dynamics and interactions

10:00-10:30 Bartosz Rozycki, Institute of Physics PAS, Warsaw, Poland

Ensembles of multi-protein complexes in simulation and experiment

10:30-11:00 Maksim Kouza, University of Warsaw, Poland

Molecular Dynamics Simulations of Forced Protein Unfolding

11:00-11:30 *Coffee Break*

Chairperson A. Kolinski

11:30-12:00 Slawomir Filipek, University of Warsaw, Poland

Activation Routes of G-Protein-Coupled Receptors

12:00-12:30 Phuong Hoang Nguyen, Institute of Biophysical Chemistry, CNRS, Paris

Structures and dynamics of Aβ oligomers and their interactions with known inhibitors

12:30-13:00 Tap Ha-Duong, University Paris-Sud, Châtenay-Malabry, France

Coarse-grained molecular modeling of the membrane receptor CXCR4 recognition by the chemokine CXCL12

13:00-14:30 **Lunch and Poster Section**

Chairperson: Phuong Hoang Nguyen

14:30-15:00 Sebastian Kmiecik, University of Warsaw, Poland

Introduction to CABS-based tools for protein modeling: CABS-flex, CABS-fold and py-CABS

15:00-15:30 Trung Hai Nguyen, Forschungszentrum Jülich GmbH, Germany

Cisplatin binding to proteins: insights from molecular simulation

15:30-16:00 Mai Suan Li, Institute of Physics PAS, Warsaw, Poland

Protein aggregation: Insights from lattice models

Saturday, 17 May 2014

From 10:00 Excursion

Remark: All posters will be viewed during the whole time of the conference. Please, place your poster immediately after arrival and dismount it not earlier than after the closing lecture.