List of Poster Presentations

(presented at Thursday, 5 March 2020 16:00-17:00)

1) **Miroslav Medved, S. Sitkiewicz, E. Matito, J. M. Luis and R. Zaleśny**

   Vibrational NLO properties of hydrogen-bonded systems: the challenge for DFT

2) **Libor Veis, Jiri Brabec and Pavel Beran**

   MOLMPS: the massively parallel quantum chemical density matrix renormalization group program

3) **Jan Brandejs, Jakub Visnak, Libor Veis, Örs Legeza, Jakub Lang, Andrej Antalik, Jiri Brabec and Jirí Pittner**

   Recent progress in the DMRG-tailored coupled cluster method: efficient DLPNO implementation and 4c-relativistic version

4) **Koen Veys and Daniel Escudero**

   Prediction of Anti-Kasha Behavior in Azulene Derivatives

5) **Dagmar Zaoralová**

   2D Chemistry: Chemical Control of Graphene Derivatization

6) **Jana Martincová**

   Oxidation of metallic transition metal dichalcogenides 1T-MoS_2 and 1T-TaS_2

7) **Masoumifeshania Emran**

   Calculation of molecular properties with systematic molecular fragmentation

8) **Stefan Vuckovic, John Kozlowski, Kieron Burke, Suhwan Song and Eunji Sim**

   Density Functional Analysis: The Theory of Density-Corrected DFT

9) **Egidius Smeets**

   Development of chemically accurate meta-GGA functionals for hydrogen reacting with transition metals.

List of Poster Presentations (continued)

10) Anna M. Wernbacher, Fabian L. Huber, Daniel Perleth, Sven Rau and Leticia González

Ruthenium water oxidation catalysts: Effect of ligand modification on their spectroscopic properties

11) Andreas Windischbacher, Larissa Egger, Georg Koller and Peter Puschnig

Electronic structure of Linear Acenes on Coinage Metal Surfaces

12) Smruti Ranjan Sahoo, S. Sharma and S. Sahu

Air-stable organic semiconductors for electronic and optical application: A theoretical study

13) Katarzyna Jakubowska and Magdalena Pecul

Nuclear Magnetic Resonance Parameters of Mercury Atom and Water

14) Michal Smialkowski and Michal Tomza

Highly polar molecules containing silver and copper atoms with alkali and alkaline earth metal

15) Florian Feyersinger, Peter Puschnig, Florian Libisch und A. Daniel Boese

Density Embedding for Organic Molecules on Surfaces