

## Preliminary program and schedule (draft 4/08/2014)

### *Sunday, August 24*

14.00 – 19.30 *Arrival and registration*

20.00 *Welcome party*

### *Monday, August 25*

9.00 – 9.20 **Opening remarks**

#### **Session 1: Atmospheric and astrochemical systems.**

**Chair: Robert Kolos (Warsaw, Poland)**

9.20 – 10.00 **Jacek Krelowski (Torun, Poland) (IL -1)**

*Observational investigations of molecular species in translucent interstellar clouds*

10.00 – 10.20 **Stephane Coussan (Marseille, France) (IT-1)**

*From water aggregates trapped in cryogenic matrices to amorphous solid water*

10.20 – 10.40 **Alexey Baklanov (Novosibirsk, Russia) (CT-1)**

*Singlet oxygen photogeneration from X-O<sub>2</sub> van der Waals complex. Double-spin flip vs. charge-transfer mechanism*

10.40 – 11.10 - *Coffee break*

#### **Session 2: Quantum hosts**

**Chair: Alexander Nemukhin (Moscow, Russia)**

11.10 – 11.50 **David Anderson (Wyoming, USA) (IL-2)**

*H-atom reactions in solid parahydrogen: a relatively unexplored strange chemical world*

11.50 – 12.30 **Yuan-Pern Lee (Taipei, Taiwan) (IL-3)**

*Infrared absorption of unstable species and protonated species in solid para-hydrogen*

12.30 – 12.50 **Vladimir Khmelenko (Texas, USA) (IT-2)**

*Studies of explosive destruction of impurity helium condensates*

**13.00 – 14.00 - Lunch**

### **Session 3: Atoms, clusters and nanoparticles**

**Chair: Tatyana Shabatina (Moscow, Russia)**

14.30 – 15.10 **R. Benny Gerber (Jerusalem, Israel/ Irvine, USA/ Helsinki, Finland) (IL-4)**

*Computational predictions of novel molecular crystals and clusters: chemical stability and structure*

15.10 – 15.30 **Dmitry Bezrukov (Moscow, Russia) (CT-2)**

*Metal atoms and dimers isolated in inert matrices: modeling of the stable trapping sites*

15.30 – 16.10 **Eugene Gordon (Chernogolovka, Russia) (IL-5)**

*Thermal stability of metallic nanowires and microspheres*

16.10 – 16.40 – *Coffee break*

**16.40 – 18.40 Poster Session 1**

**19.00 – 20.00 – Dinner**

***Tuesday, August 26***

### **Session 4: Chemical reactions at low temperatures**

**Chair: Vladimir Feldman (Moscow, Russia)**

9.00 – 9.40 **Wolfram Sander (Bochum, Germany) (IL – 6)**

*Tunneling reactions in low temperature matrices*

9.40 – 10.20 **Claudine Crepin-Gilbert (Paris, France) (IL-7)**

*Stimulated emission in tetrapyrrolic molecules trapped in low temperature matrices*

10.20 – 10.40 **Kenji Takahashi (Kanazawa, Japan) (IT-3)**

*Solvation dynamics of excess electrons in low temperature ionic liquid*

10.40 – 11.10 – *Coffee break*

11.10 – 11.50 **Jian-Ping Zhang (Beijing, China) (IL-8)**

*Ultrafast dynamics of charge photogeneration in polymer solar cells*

11.50 – 12.10 **Oleg Shlyakhtin (Moscow, Russia) (IT-4)**

*Current trends in the freeze drying synthesis and cryoprocessing of inorganic materials*

12.10 – 12.30 **Anatoliy Pukhovskiy (Moscow, Russia) (IT-5)**

*Long-term structure investigations of chlorine atom – arene complexes: epistemological aspects*

12.30 – **Group photo**

**13.00 – 14.00 – Lunch**

### **Session 5: Young Investigators Session**

**Chair: Mika Pettersson (Jyväskylä, Finland)**

15.00 – 15.15 **Claudio Nunes (Coimbra, Portugal) (YIS-1)**

*Generation and reactions of nitrile and nitrile imines induced by tunable UV- light*

15.15 - 15.30 **Sergey Ryazantsev (Moscow, Russia) (YIS-2)**

*Matrix isolation studies on the radiation-induced processes in H<sub>2</sub>O/CO<sub>2</sub> system*

15.30 – 15.45 **Jaroslav Kalinowski (Helsinki, Finland) (YIS-3)**

*Nature, isomerization and decomposition of a Criegee intermediates: dynamics using a multireference potential*

15.45 – 16.00 **Maria Khrenova (Moscow, Russia) (YIS-4)**

*Theoretical characterization of intermediates of photocycle of Bluf receptor observed at low temperatures*

16.00 – 16.15 **Alexander Bogomolov (Novosibirsk, Russia) (YIS-5)**

*Predissociation of high-lying Rydberg states of molecular iodine via ion-pair state*

16.15 – 16.30 **Ivan Sorokin (Moscow, Russia) (YIS-6)**

*Photochemical transformations of the 1,4-dithiane radical cation: a novel approach to conformational isomerization of reactive intermediates in freonic matrices*

16.30 – 17.00 **Coffee break**

**17.00 – 19.00 – Free time**

**19.00 – Dinner**

**Wednesday, August 27**

### **Session 6: Reactive intermediates and novel species**

**Chair: Joelle Mascetti (Bordeaux, France)**

9.00 – 9.40 **Eugene Misochko (Chernogolovka, Russia) (IL-9)**

*Matrix-isolated triplet diradicals with strongly delocalized unpaired electrons: ESR spectroscopy and quantum chemical calculations*

9.40 – 10.00 **Anton Savitsky (Berlin, Germany) (IT-6)**

*Carbene and solvation: an advanced EPR study*

10.00 – 10.20 **Alexander Akimov (Chernogolovka, Russia) (CT-3)**

*High-spin organic radicals with large spin-orbit contribution to zero-field splitting constant: X- and W-band EPR studies*

10.20 – 10.50 – *Coffee break*

### **Session 7: Systems of biological interest and medical applications**

**Chair: György Tarczay (Budapest, Hungary)**

10.50 – 11.30 **Tigran Kurtikyan (Erevan, Armenia) (IL-10)**

*Interaction of nitrogenoxides with heme models. Low temperature spectral characterization of biologically important intermediates*

11.30 – 11.50 **Igor Reva (Coimbra, Portugal) (IT-7)**

*Light-induced processes in matrix-isolated cytosines*

11.50 – 12.10 **Alexander Nemukhin (Moscow, Russia) (IT-8)**

*Molecular mechanisms of xenon anesthesia: A link to low-temperature studies of xenon complexes*

12.10 – 12.50 **Vladimir Lozinsky (Moscow, Russia) (IL-11)**

*Poly(vinyl alcohol)cryogels – materials of the XXI century, and how the composition of initial feed and freeze-thaw regimes can affect the properties and macroporous morphology of these cryochemical products*

12.50 – 13.10 **Yuri Morozov (Moscow, Russia) (CT-4)**

*Cryochemistry for drugs nanoform synthesis*

**13.15 – 14.15 – Lunch**

**14.30 – 18.00 – Excursion**

**19.00 – 20.00 - Dinner**

**Thursday, August 28**

### **Session 8: Spectroscopy and dynamics in matrices – Marilyn Jacox Memorial Session**

**Chair: Markku Räsänen (Helsinki, Finland)**

9.00 – 9.40 **Rui Fausto (Coimbra, Portugal) (IL-12)**

*A low temperature spectroscopy investigation of the intermolecularly-induced conformational disorder in ferrocene derivatives*

9.40 – 10.20 **Leonid Khriachtchev (Helsinki, Finland) (IL-13)**

*Matrix-isolation studies of non-covalent interactions: more sophisticated approaches*

**10.20 – 10.50 – Coffee break**

10.50 - 11.30 **Tomonari Wakabayashi (Osaka, Japan) (IL-14)**

*Spectroscopy of linear polyyne molecules and bismuth clusters*

11.30 – 12.10 **Mika Pettersson (Jyväskylä, Finland) (IL-15)**

*Raman spectroscopic studies of matrix isolated species*

12.10 – 12.40 – **Business meeting**

12.40 – 12.50 **Closing remarks**

**13.00 – 14.00 – Lunch**

**15.00 – 17.00 – Poster session 2**

**17.00 – 19.00 – Free time**

**19.00 – Conference Dinner (Banquet)**

**Friday, August 29**

9.00 – 10.00 - **Departure**