

# PROGRAMME

of the International workshop

## Applications of topological methods in materials science

**Friday, July 1<sup>st</sup>, SCTMS conference hall**

9<sup>00</sup>-9<sup>15</sup> Welcome and Introduction

**Morning session.** Chairman **Prof. Vladislav Blatov**, Samara Center for Theoretical Materials Science (Samara, Russia)

9<sup>15</sup>-10<sup>15</sup> **Prof. Jean-Guillaume Eon**, Federal University of Rio de Janeiro (Brazil) “*Topological Features in Crystal Structures: a Quotient Graph-Assisted Analysis of Underlying Nets and their Embeddings*”

10<sup>15</sup>-11<sup>15</sup> **Dr. Peter G. Boyd**, École Polytechnique Fédérale de Lausanne (Switzerland) “*A Novel Method for Constructing Nano Porous Materials from Labelled Quotient Graphs*”

11<sup>15</sup>-11<sup>30</sup> Coffee break

11<sup>30</sup>-12<sup>30</sup> **Dr. Matthew Addicoat**, University of Leipzig (Germany) “*Computational prediction of MOF structures from the entire periodic table: AuToGraFS + UFF4MOF*”

12<sup>30</sup>-13<sup>45</sup> Lunch

**Afternoon session.** Chairman **Prof. Davide Proserpio**, University of Milan (Italy)

13<sup>45</sup>-14<sup>45</sup> **Dr. Felipe Gándara**, Materials Science Institute of Madrid (Spain) “*Preparation and Properties of Group-13 and Solid-Solution Metal-Organic Framework*”

14<sup>45</sup>-15<sup>30</sup> **Dr. Jian Lu**, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences (China) “*Porphyrim-Based Supramolecular Organic Frameworks: Storage and Separation*”

15<sup>30</sup>-15<sup>45</sup> Coffee break

15<sup>45</sup>-16<sup>30</sup> **Dr. George Kostakis**, University of Sussex (UK) “*3d/4f Coordination Clusters in Catalysis*”

16<sup>30</sup>-17<sup>15</sup> **Dawid Bednarski**, University of Hamburg (Germany) “*Topologically interesting Materials from Hamburg. 'Reticular' synthesis with unexpected/surprising results*”

17<sup>15</sup>-18<sup>00</sup> **Dr. Ruggero Gabbrielli**, Istituto Tecnico Industriale Statale Nullo Baldini (Ravenna, Italy) “*Periodic partitions and aggregates of similarly-sized bubbles*”

**Saturday, July 2<sup>nd</sup>, SCTMS conference hall**

**Morning session.** Chairman **Prof. Jean-Guillaume Eon**, Federal University of Rio de Janeiro (Brazil)

9<sup>00</sup>-9<sup>45</sup> **Prof. Davide Proserpio**, University of Milan (Italy) “*Entanglement in 2-Periodic Coordination Networks*”

9<sup>45</sup>-10<sup>30</sup> **Prof. Vladislav Blatov**, Samara Center for Theoretical Materials Science (Samara, Russia)  
“*Topological methods in ToposPro*”

10<sup>30</sup>-10<sup>45</sup> Coffee break

10<sup>45</sup>-11<sup>30</sup> **Prof. Vladimir Saleev**, Samara Center for Theoretical Materials Science (Samara, Russia) “*New  $sp^3$  silicon and germanium allotropes from the topology-based multiscale method*”

11<sup>30</sup>-12<sup>00</sup> **Dr. Alexandra Shipilova**, Samara Center for Theoretical Materials Science (Samara, Russia)  
“*From zeolite nets to low-energy  $sp^3$  carbon allotropes with 3- and 4-rings using the hybrid topological-quantum mechanical method*”

12<sup>00</sup>-12<sup>30</sup> **Gulshan Kumar**, University Delhi (India) “*Coordination-Driven Frameworks Using Molecular Building Blocks*”

12<sup>30</sup>-14<sup>00</sup> Lunch

**Afternoon session.** Chairman **Dr. George Kostakis**, University of Sussex (UK)

14<sup>00</sup>-14<sup>30</sup> **Dr. Eugeny Alexandrov**, Samara Center for Theoretical Materials Science (Samara, Russia)  
“*Topological collections, Knowledge bases, and Expert systems in crystal chemistry*”

14<sup>30</sup>-15<sup>00</sup> **Dr. Roman Eremin**, Samara Center for Theoretical Materials Science (Samara, Russia)  
“*Combined topological/density functional theory analysis for potential potassium ion conducting materials*”

15<sup>00</sup>-15<sup>20</sup> **Dr. Muhammad Ali Butt**, Samara National Research University (Samara, Russia) “*Growth of single  $RbTiOPO_4$  crystal and epitaxial layers*”

15<sup>20</sup>-15<sup>40</sup> **Pavel Zolotarev**, Samara Center for Theoretical Materials Science (Samara, Russia) “*Descriptors of anisotropy of intermolecular interactions in organic molecular crystals*”

15<sup>40</sup>-15<sup>50</sup> Coffee break

15<sup>50</sup>-16<sup>10</sup> **Andrey Golov**, Samara Center for Theoretical Materials Science (Samara, Russia) “*Application of Voronoi partition for analysis of porous materials*”

16<sup>10</sup>-16<sup>30</sup> **Andrey Goltsev**, Samara Center for Theoretical Materials Science (Samara, Russia) “*Rod packings in coordination polymers*”

16<sup>30</sup>-16<sup>50</sup> **Tatiana Akhmetshina**, Samara Center for Theoretical Materials Science (Samara, Russia)  
“*Topological analysis of icosahedron-based intermetallics*”

16<sup>50</sup>-18<sup>00</sup> Flash presentation from participants of the workshop, 5 minutes each

18<sup>00</sup>-18<sup>15</sup> Closing remarks