

PROGRAMME

of the International Scientific School

Combined topological and DFT methods for prediction of new materials II

Monday, July 04th, SCTMS conference hall

9⁰⁰-9¹⁵ Welcome and Introduction

9¹⁵-10⁴⁵ V.A. Blatov, Lecture “Computer crystallochemical analysis: an introduction”

10⁴⁵-11⁰⁰ Coffee break

11⁰⁰-12³⁰ V.A. Blatov, D.M. Proserpio, Exercises “Introduction to ToposPro”

12³⁰-14⁰⁰ Lunch

14⁰⁰-15³⁰ V.A. Blatov, D.M. Proserpio, Exercises “Visualization of 0D, 1D, 2D and 3D structures”

15³⁰-15⁴⁵ Coffee break

15⁴⁵-17¹⁵ V.A. Blatov, Lecture “Methods, software, databases, and expert systems for crystallochemical analysis”

17¹⁵-18⁰⁰ Q&A

Tuesday, July 05th, SCTMS conference hall

9⁰⁰-10³⁰ D.M. Proserpio, Lecture “Graphs, nets, and tilings- I”

10³⁰-10⁴⁵ Coffee break

10⁴⁵-12¹⁵ D.M. Proserpio, Lecture “Graphs, nets, and tilings- II”

12¹⁵-14⁰⁰ Lunch

14⁰⁰-15³⁰ V.A. Blatov, D.M. Proserpio, Exercises “Standard methods of simplification of crystal structures”

15³⁰-15⁴⁵ Coffee break

15⁴⁵-17¹⁵ V.A. Blatov, D.M. Proserpio, Exercises “Special methods of simplification of crystal structures”

17¹⁵-18⁰⁰ Q&A

Wednesday, July 06th, SCTMS conference hall

9⁰⁰-10³⁰ D.M. Proserpio, Lecture “Topological analysis of entanglements”

10³⁰-10⁴⁵ Coffee break

10⁴⁵-12³⁰ V.A. Blatov, D.M. Proserpio, Exercises “Topological identification of nets. Working with the TTD collection, Systre, and SCTMS Online Services”

12³⁰-14⁰⁰ Lunch

14⁰⁰-15³⁰ V.A. Blatov, D.M. Proserpio, Exercises “Visualization, topological analysis and classification of MOFs and coordination polymers”

15³⁰-15⁴⁵ Coffee break

15⁴⁵-17¹⁵ V.A. Blatov, D.M. Proserpio, Exercises “Visualization, topological analysis and classification of entangled networks”

17¹⁵-18⁰⁰ Q&A

19⁰⁰ Social Dinner

Thursday, July 07th, SCTMS conference hall

9⁰⁰-10³⁰ V.A. Blatov, D.M. Proserpio, Exercises “Computing natural tilings and their parameters with ToposPro. Analysis of zeolites and fast-ion conductors”

10³⁰-10⁴⁵ Coffee break

10⁴⁵-12³⁰ V.A. Blatov, D.M. Proserpio, Exercises “Working with Systre and 3dt programs”

12³⁰-14⁰⁰ Lunch

14⁰⁰-15³⁰ V.A. Blatov, D.M. Proserpio, Exercises “Nanocluster representation of intermetallic compounds”

15³⁰-15⁴⁵ Coffee break

15⁴⁵-17¹⁵ V.A. Blatov, E.V. Alexandrov, Exercises “Creating knowledge databases for crystal chemistry and materials science”

17¹⁵ -18⁰⁰ Q&A

Friday, July 08th, SCTMS conference hall

9⁰⁰-10³⁰ D.M. Proserpio, Lecture “The topological approach to crystal chemistry: An historical account”

10³⁰-10⁴⁵ Coffee break

10⁴⁵-12³⁰ V.A. Saleev, Lecture “DFT as a basis of modern theoretical materials science”

12³⁰-14⁰⁰ Lunch

14⁰⁰-15³⁰ A.V. Shipilova, “Introduction to VASP”

15³⁰-15⁴⁵ Coffee break

15⁴⁵-17¹⁵ A.V.Shipilova, Exercises “Running VASP- I”

17¹⁵ -18⁰⁰ Q&A

Saturday, July 09th, SCTMS conference hall

9⁰⁰-10³⁰ A.V. Shipilova, Lecture “Hybrid topological-DFT methods for the prediction of new materials”.

10³⁰-10⁴⁵ Coffee break

10⁴⁵-12³⁰ A.A. Kabanov, Lecture “Topological analysis of ionic conductivity in solids”.

12³⁰-14⁰⁰ Lunch

14⁰⁰-15³⁰ A.A. Kabanov, Exercises “DFT and topological investigations of ionic conductivity in solids”

15³⁰-15⁴⁵ Coffee break

15⁴⁵-17¹⁵ R.A. Eremin, Exercises “Exploring ionic conductivity using CP2K package”

17¹⁵ -18⁰⁰ Q&A

Sunday, July 10th, SCTMS conference hall

9⁰⁰-10³⁰ A.V.Shipilova, A.A. Kabanov, Exercises “Running VASP - II”

10³⁰-10⁴⁵ Coffee break

10⁴⁵-12¹⁵ V.A. Blatov, D.M. Proserpio, V.A. Saleev, Exercises “Solving individual tasks based on the participants' own structures”

12¹⁵-12³⁰ Summary and Conclusions