## **GI-MS45-P01** | **C**RYSTALLOCHEMICAL COMPUTATIONAL TOOLS, WEB SERVICES, DATABASES,

## AND APPROACHES FOR JOINING RESEARCHERS OVER THE WORLD

Alexandrov, Eugeny V. (Samara Center for Theoretical Materials Science (SCTMS), Samara University, Samara, RUS); Proserpio, Davide M. (Dipartimento di Chimica, Università degli Studi di Milano, Samara, RUS); Blatov, Vladislav A. (Samara Center for Theoretical Materials Science (SCTMS), Samara State Technical University, Samara, RUS); Addicoat, Matthew (Nottingham Trent University, School of Science and Technology, Nottingham, AUT)

The Samara Center for Theoretical Materials Science (SCTMS) started in 2013 from one successful collaboration (http://english.sctms.ru/about/) and then the collaboration network was enlarged to more than 15 countries, 30 groups, and 100 researchers. The approaches for geometrical-topological analysis (https://topospro.com/; https://topcryst.com/) developed in SCTMS cover crystal chemistry of almost all classes of crystalline materials [1-3]. Use of them in couple with knowledge-based approach results in establishing structures taxonomy, finding correlations between structural descriptors, and predicting structures and properties on a qualitative level [4,5]. We see three conditions to be crucial for a long, stable and fruitful collaboration: (i) a rigorously defined scientific task, (ii) flexibility and diversity of research interests, and (iii) development in line with modern trends in science.

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