



# Computational Materials Science Center

## Student workshop

### Computational methods in molecular and solid-state systems

10:00 - 10:10 Introduction (Estela Blaisten-Barojas)

10:10 - 10:50 Computational geometry of molecular structure (Iosif Vaisman)

10:50 - 11:20 Computational analysis of mineral structure (Shujiang Yang)

11:20 - 11:50 Structure visualization (Mohamed Lach-Hab and Daniel Carr)

11:50 - 12:30 Lunch break

12:30 - 2:30 Machine learning methods (Majid Masso)

2:30 - 3:30 Crystallographic and bioinformatics structure analysis in macromolecular complexes (Eugene Krissinel)

#### Acknowledgments:

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# SAMP: Structure-Adaptive Materials Prediction

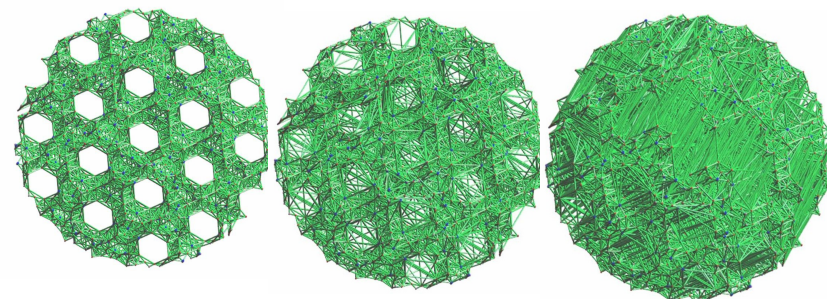
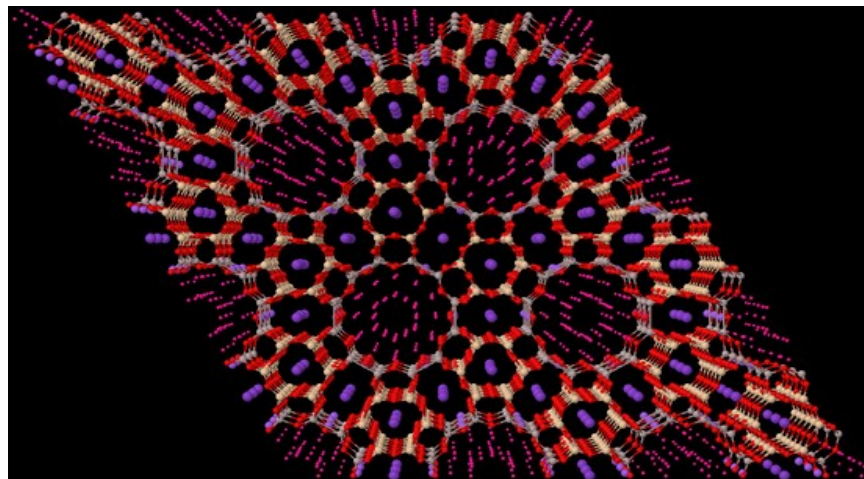
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Intelligent data mining tools and materials design strategies using crystallographic and materials property data sources can be enriched by developing a rational cyber-design for determining the nature and types of data equivalencies in the structural chemical information of materials. A visual portal enhancing the use of intelligently organized correlations of structural chemical data for predicting better or new materials will be applied within a Web-based learning system for educational and development purposes. This approach will be tested in several graduate and undergraduate chemical courses.

We developed a novel knowledge-based approach to the zeolite structure classification and prediction. The methodology is based on computational geometry analysis of topology in the training set of known zeolite structures and it incorporates machine learning tools to build a structure classification model. Currently, the preliminary model for 40 classes can be used for zeolite crystal assignment with high accuracy, ranging from 90 to 97% depending on the model type and number of parameters.



Delaunay tessellated spherical fragment of the zeolite crystal shown above used for the model construction as a function of simplex edge length: left atomic scale, right nanometer scale