

8th USPEX Workshop

January 20-24, 2015

Organizers:

Priya Johari (Shiv Nadar University, India; priya.johari@snu.edu.in)

Artem R. Oganov (Stony Brook University, USA; artem.oganov@stonybrook.edu)

Sayed Faheem Naqvi (Anand International College of Engineering, Jaipur, India)

Hosted by

*The Department of Physics, School of Natural Sciences, Shiv Nadar University,
Greater Noida, U.P. – 201301. INDIA*

Supporting Organizations

Shiv Nadar University

Stony Brook University

International Union of Crystallography

Day Plan

DAY 1.

G. Desiraju "Computational crystallography and materials of the future"

A.R.Oganov "Crystal structure prediction and the USPEX code"

Q. Zhu "Prediction of the structure of molecular crystals"

TUTORIALS:

-tutorial on data analysis (D. Dong)

-prediction of high-pressure phases (A.R. Oganov)

-molecular crystals (Q. Zhu)

DAY 2.

S.L. Chaplot "Novel materials at high-pressure"

Q. Zhu "Variable-composition evolutionary structure prediction"

Q.F. Zeng "Optimization of physical properties"

TUTORIALS:

-variable-composition structure predictions (G.R. Qian)

-optimization of physical properties (A.R. Oganov)

DAY 3.

Excursion: Agra and Taj Mahal.

DAY 4.

P. Johari "Theory and simulations of low-dimensional systems"

Q. Zhu "Evolutionary structure prediction for nanoparticles and surfaces"

C.H. Hu "Applications of that variable-composition structure prediction"

TUTORIALS:

-nanoparticles and surfaces (X.-F. Zhou)

DAY 5.

A.R. Oganov "Evolutionary metadynamics"

G.R. Qian "Methods for predicting phase transition mechanisms: variable-cell nudged elastic band method and transition path sampling"

2-3 TALKS OF THE PARTICIPANTS

TUTORIALS:

-evolutionary metadynamics (A.R. Oganov)

-variable-cell NEB method (G.R. Qian)

How to apply

The number of participants from outside SNU will be limited to 50 – so apply early. All participants should register for USPEX code at <http://uspex.stonybrook.edu/uspexdownloads.php> before applying.

Interested candidates should register at www.snu.edu.in/uspex.aspx and pay the registration fee. The payment can be made through demand draft in favor of “Shiv Nadar University” payable at Noida.

International candidates will have to pay on-site. **Those interested in receiving financial support should send their CV and list of publications, if any, to the e-mail: uspex.2015@snu.edu.in before October 15, 2014.** Selected participants will be notified by **October 31, 2014.**

Registration fees:

	Early Bird (Before Nov' 15, 2014)	Late (Between Nov' 15 and Dec' 15, 2014)
UG and PG students / Research Scholars	Rs. 3,500/-	Rs. 4,500/-
Academia / R&D Institutions	Rs. 6,500/-	Rs. 7,500/-
Industry	Rs. 10,500/-	Rs. 11,500/-

Note: For industry USPEX is not free, so before coming to workshop they should buy license.

Financial Support:

Selected participants will be given accommodation in SNU hostels and provided with local hospitality.