International Workshop “Evolutionary crystal structure prediction using the USPEX code: discovery of new materials and mineral phases”
(USPEX 2011 Xi’an)

August 2-6, 2011
Xi’an, China
ABOUT THE WORKSHOP
Crystal structure prediction, until recently thought to be fundamentally impossible, has now become a topic of intense research. Applications are found in computational materials design, study of materials at high pressure, discovery of new mineral phases in planetary interiors, and fundamental studies of chemical bonding and structure-property relations. This field opens vast horizons for the discovery of novel materials for virtually all types of applications. The great progress made recently happened largely thanks to the development of the USPEX method/code, which is now used by over 500 researchers around the world. This workshop aims to bring together the developers of USPEX and its users, as well as anyone interested in crystal structure prediction and computational materials design.

USPEX 2011 XI’AN TOPICS
1. Crystal structure prediction: problem and possible solutions
2. USPEX code: theory and hands-on tutorials
3. Visualization and analysis of large structural datasets
4. Energy landscapes: concept and applications in structure prediction
5. Structure prediction for nanoparticles and surfaces
6. Search for materials with target properties
7. Small research projects in crystal structure prediction

USPEX 2011 XI’AN ORGANIZATION
USPEX 2011 Xi’an Organizers
Stony Brook University (SBU), USA
Northwestern Polytechnical University (NWPU), China
USPEX 2011 Xi’an Endorsers
National Key Lab of Thermostruct. Composite Mater. (NKLTSCM), NWPU, China
International Cooperation Office, NWPU, China
111 project base of NWPU, China
Department of Geosciences, SBU, USA
Beijing Hongcam Company, China
USPEX 2011 Xi’an Co-chairs
Artem R. Oganov (SBU, USA)
Laifei Cheng (NWPU, China)
Qingfeng Zeng (NWPU, China)
Tian Cui (Jilin University (JU), China)
USPEX 2011 Xi’an Secretary
Zuohai Weng, NKLTSCM, NWPU, China
USPEX 2011 Xi’an Invited Speakers
Artem R. Oganov (Stony Brook University, USA)
Mario Valle (Swiss Supercomputer Centre, Switzerland)
Tian Cui (Jilin University, China)
Zhiqiang Feng (Université d’Evry, France)
Gilles Frapper (University of Poitiers, France)
Chaohao Hu (Guilin University of Electronic Technology, China)
Andriy O. Lyakhov (Stony Brook University, USA)
Qingfeng Zeng (Northwestern Polytechnical University, China)
REGISTRATION

Tuesday, August 2, 2011
9:00-18:00 Registration at the ground floor, Kairui Hotel
Registration fee: (Accommodation & Meals1; tour)
Nonacademic participants: 500USD/person (3200 CNY);
Academic participants: 400USD/person (2600 CNY);
Students: 300USD/person (2000 CNY);
Families: 200USD/person (1300 CNY);
Exhibition: 1000USD/site (6000 CNY).
Invited speakers are free for registration fee, supported by other funds.

TECHNICAL PROGRAM

Tuesday, August 2, 2011
19:30 Welcoming banquet at the 2nd floor, Kairui Hotel

Wednesday AM, August 3, 2011
08:20 Opening Ceremony
Chaired by Qingfeng Zeng
Laifei Cheng (Director of NKLTSCM, NWPU, China)
Artem Oganov (Main developer of USPEX, SBU, USA)

Photo in front of the library

Presentation session I
09:00 Crystal structure prediction
Artem R. Oganov (Stony Brook University, USA)
09:40 Searching for new high-pressure phases
Tian Cui (Jilin University, China)
10:20 Coffee Break

Presentation session II
Chaired by Artem Oganov
10:40 Extending the USPEX algorithm: large systems, variable composition, nanoparticles
Andriy O. Lyakhov (Stony Brook University, USA)
11:20 Solid chlorine under pressure
Weiwei Zhang (China Agricultural University, China)
12:00 Buffet lunch at the 2nd floor, Zhenghe Hotel

Wednesday PM, August 3, 2011
Practical session I
Chaired by Qiang Zhu
14:00 How to predict high-pressure crystal structures
Artem R. Oganov (Stony Brook University, USA)

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1 Accommodation & Meals, 5 days from 2nd to 7th August; accommodation for extra day is 200CNY/day, paid at the front desk of the hotel, the remaining is supported from other funds.
16:00 Coffee Break
16:20 (continue)
   Artem R. Oganov (Stony Brook University, USA)
18:20 From unsatured molecules to extended systems: searching for novel materials
   Gilles Frapper (University of Poitiers, France)
19:00 Dumpling Dinner at City Center

Thursday AM, August 4, 2011
Presentation Session III
Chaired by Tian Cui
08:20 Hydrogen-rich systems under pressure
   Chaohao Hu (Guilin University of Electronic Technology, China)
09:00 Fingerprint theory
   Mario Valle (Swiss Supercomputer Centre, Switzerland)
09:40 Structure prediction for molecular crystals
   Qiang Zhu (Stony Brook University, USA)
10:20 Coffee Break

Presentation Session IV
Chaired by Zhiqiang Feng
10:40 Structure prediction using USPEX: a user’s experience
   Xiang-Feng Zhou (Nankai University, China)
11:20 Computational phase diagram: post-USPEX
   Qingfeng Zeng (Northwestern Polytechnical University, China)
12:00 Buffet lunch at the 2nd floor, Zhenghe Hotel

Thursday AM, August 4, 2011
Practical session II
Chaired by Qiang Zhu
14:00 Visualization of crystal structures and analysis of USPEX data
   Mario Valle (Swiss Supercomputer Centre, Switzerland)
16:00 Coffee Break
Practical session III
Chaired by Andriy O. Lyakhov
16:20 Hydrogen-rich systems under pressure
   Chaohao Hu (Guilin University of Electronic Technology, China)
18:20 Round table & Student presentation
   First-principles-based study of temperature effects in perovskite ferroelectrics
   Nikita Matsko (P.N. Lebedev Physical Institute, Russian Academy of Sci., Russia)
19:00 BBQ at Le Garden Hotel

Friday AM, August 5, 2011
Presentation session V
Chaired by Chaohao Hu
08:20 Computational modeling for materials and structures: scale beyond atoms
   Zhiqiang Feng (Université d'Evry, France)
Practical session IV  
Chaired by Mario Valle  
09:00  How to deal with variable-composition systems  
Weiiwei Zhang (China Agricultural University, China)  
10:20  Coffee Break  

Practical session V  
Chaired by  
10:40  How to predict the structure of nanoparticles  
Andriy O. Lyakhov (Stony Brook University, USA)  
Qiang Zhu (Stony Brook University, USA)  
12:00  Award and closing ceremony at NKLTSCM  
12:30  Lunch at Dongfang Restaurant  

14:00-21:00 Shaanxi Historic Museum, Wide Goose Pagoda Square & Tang Paradise  

Saturday AM, August 6, 2011  
08:30-21:00 Tour of Xi’an and surroundings  
Terracotta Army & Xi’an Horticulture Expo  

WORKSHOP VENUE  
USPEX 2011 Xi’an will be held on August 2–6, 2011, at Yizilou, NWPU, Xi’an, China. During the workshop, the USPEX OFFICE will be located in Kairui Hotel, Xi’an.  

SPECIAL EVENTS  
Welcoming Banquet  
On Tuesday evening, August 2, 2011, from 19:30 to 21:00, the welcoming banquet is planned for USPEX participants and their guests at the 2nd floor, Kairui Hotel. The banquet fee is free.  
Award and Closing Ceremony  
On Friday noon, August 5, 2011, from 12:00 to 12:30, winner of each practical session will receive a recent book “Modern Methods of Crystal Structure Prediction” with the signature of Prof. Artem R. Oganov and the stamp of NKLTSCM.  

ACCOMMODATION  
The Le Garden Hotel and Kairui Hotel provide various rooms for the participants. Workshop will cover accommodation fee for 5 days from 2nd to 7th August. Accommodation for an extra day is 200CNY/day, paid at the front desk of the hotel, the remaining is supported from other funds. The accommodation fee for the invited speakers is free during the workshop. The families accompanied should pay the fee if they need additional rooms.
## SUMMARY OF THE PROGRAM

<table>
<thead>
<tr>
<th>Time</th>
<th>2 Aug Tue</th>
<th>3 Aug Wed</th>
<th>4 Aug Thu</th>
<th>5 Aug Fri</th>
<th>6 Aug Sat</th>
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<tbody>
<tr>
<td>8:20-9:00</td>
<td>Arrival &amp; Registration</td>
<td>Opening ceremony</td>
<td>Chaohao Hu “Hydrogen-rich systems under pressure”</td>
<td>ZhiQiang Feng “Computational modeling for materials and structures: scale beyond atoms”</td>
<td>Terracotta Army &amp; Xi’an Horticulture Expo</td>
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<td>9:00-9:40</td>
<td>Artem R. Oganov “Crystal structure prediction”</td>
<td>Mario Valle “Fingerprint theory”</td>
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<td>Practical Session IV Weiwei Zhang</td>
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<td>9:40-10:20</td>
<td>Tian Cui “Searching for new high-pressure phases”</td>
<td>Qiang Zhu “Structure prediction for molecular crystals”</td>
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<td>10:20-10:40</td>
<td>Coffee</td>
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<td>10:40-11:20</td>
<td>Andriy O. Lyakhov “Extending the USPEX algorithm: large systems, variable composition, nanoparticles”</td>
<td>Xiang-Feng Zhou “Structure prediction using USPEX: a user’s experience”</td>
<td>Practical Session V Andriy O. Lyakhov, Qiang Zhu</td>
<td>Award at the National Key Lab (12:00-12:20)</td>
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<td>11:20-12:00</td>
<td>Weiwei Zhang “Solid chlorine under pressure”</td>
<td>Qingfeng Zeng Computational phase diagram: post-USPEX</td>
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<td>12:00-14:00</td>
<td>LUNCH</td>
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<td>Practical Session I Artem R. Oganov</td>
<td>Practical Session II Mario Valle “Visualization of crystal structures and analysis of USPEX data”</td>
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<td>16:20-18:20</td>
<td>Session I (cont.) Artem R. Oganov</td>
<td>Practical Session III Chaohao Hu</td>
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<td>18:20-19:00</td>
<td>Gilles Frapper “Searching for novel materials”</td>
<td>Round table &amp; Student show (Nikita Matsko et al)</td>
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<td>19:00-21:00</td>
<td>Welcoming banquet</td>
<td>Dumpling Dinner</td>
<td>BBQ party</td>
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HOW TO GET YOUR DESTINATION

Step 1: Arriving Xi’an
Step 2: Arriving NWPU and the Hotels

Route details:

Start 1: Xi’an Xianyang International Airport
First: Walk to the Airport bus stop. Take the Airport bus line five to Xi’an Xishaomen; the bus comes from 6:00--18:30 every 20min, or Line one to Xi’an Bell Tower (Xi’an Meloen Hotel), from 6:00--20:00 every 20min, 37.4km/50min, 26CNY.
Second: Take No. 206 or 29 bus to NWPU (South Gate, near to Kairui Hotel), 201 to NWPU (West Gate, near to Le Garden Hotel), 4.8km/30min, 1CNY. You can also call a tax, and it will cost you about 10 CNY (13CNY) from XiShaomen (Bell tower).

Destination: NWPU

Start 2: North Railway Station (High speed train station)
First: Take 264 bus to Laodong Road (The end), 15km/70min, 1 CNY.
Second: And then take 24 bus to NWPU, 3.9km/20min, 1 CNY, or you can call a tax and 10CNY is enough.

Destination: NWPU

Start 3: Xi’an Railway Station
Take No. 206 or 40 bus to NWPU (South Gate), 8.2km/40min, go ahead about 50 meters, and NWPU (South Gate) is on your right.
Destination: NWPU

GENERAL INFORMATION

LANGUAGE
The official language for the Workshop is English. However, in the public society, Chinese mandarin is commonly spoken.

CURRENCY AND CREDIT CARDS
Chinese currency is CNY with its monetary unit CNY (Yuan). The exchange rate is 1 USD for about 6.5 CNY. The credit cards and cash in US dollars are acceptable at the hotel registration desk in USPEX 2011 Xi’an Host Hotel. This is also the case in most large shopping centers and other hotels.

TAX AND TIP
Tipping is by no means a traditional Chinese custom. Please help keep the good custom and do not tip a waiter/waitress or a taxi driver and other persons who provide regular service. Take back any change that is rightfully yours. All advertised prices include tax. Bargaining is quite common on buying merchandise especially from Street Markets.

TAXI
Usually, a taxi is available along the roadsides, while you wave for it. However, on main streets it is only available at taxi stops or in front of a hotel.

BUSINESS OPENING HOURS
• Bank and Post Office
  Opening hours: 9:00 – 17:00, from Monday to Sunday.
• Government Office
  Opening hours: 8:00 – 17:00, from Monday to Friday.
• Stores
  Opening hours: usually 10:00 to 21:00, but large shopping centers serve till 22:00, from Monday to Sunday.

ELECTRICITY
In China, the standard outlets provide AC of 220 V/50 Hz.