

Day 1. August 20.

- 9:00-9:15 Welcome 10th USPEX workshop – A.R. Oganov & Y.L. Li
9:15-10:15 A.R. Oganov "Crystal structure prediction and the USPEX code"
10:15-11:00 T.Cui "New hydrides and novel superconductivity under high pressures"
11:00-11:15 Tea break
11:15-12:00 Y.L. Li "Exotic stable calcium carbides: theory and experiment".
12:00-12:45 Q.F. Zeng "Optimization of physical properties using USPEX"
12:45-14:30 LUNCH
14:30-14:45 H.F. Dong "Can C-N compounds be harder than diamond?"
14:45-15:00 D. Dong TBA
15:00-16:30 TUTORIAL 1: Installation party – First steps with USPEX (Qiang Zhu, Dong Dong, Guangrui Qian, Zahed Allahyari).
16:30-19:00 TUTORIAL 2: Predicting high-pressure phases with USPEX (Artem R. Oganov, Dong Dong and Huafeng Dong)
19:00 DINNER

Day 2. August 21.

- 9:00-10:00 A.R. Oganov "Variable-composition searches for new compounds"
10:00-10:30 W.W. Zhang "Unexpected stable sodium chlorides: challenge to classical chemistry"
10:30-11:00 Tea break and group photo
11:00-11:30 S.Y. Yu "Novel chemistry found by variable-composition USPEX searches"
11:30-12:00 H.Y. Niu "Novel stable compounds in the Mg-Si-O system under extraplanet pressures"
12:00-12:30 J.J. Wang TBA
12:30-14:30 LUNCH
14:30-15:00 X. Dong "Electronegativity of elements under pressure: key to understanding novel chemistry"
15:00-15:30 Short talks of users, oral posters.
15:30-17:00 Poster session.
17:00-19:00 TUTORIAL 3: Variable-composition structure prediction (Qiang Zhu and Artem R. Oganov).
19:00 Dinner

Day 3. August 22.

- 9:00-10:00 Q. Zhu "Predicting structures of molecular crystals and polymers"
10:00-11:00 G. Frapper "A chemist's view of bonding in crystals: from molecular to extended systems".
11:00-11:15 Tea break
11:15-12:00 S. Jenkins "New understanding of chemical bonding in solids"
12:00-12:30 Q.G. Wang "Clarifying TiO₂ surfaces and transition metal carbide

crystals by USPEX"
12:30-14:30 LUNCH
14:30-15:15 Q. Zhu "Prediction of low-dimensional systems: surface reconstructions and structures of nanoparticles"
15:15-16:00 X.F. Zhou "Applications of USPEX to surfaces and 2D-crystals"
16:00-17:00 Poster session
17:00-19:00 TUTORIAL 4: Prediction of molecular crystal structures (Qiang Zhu, Dong Dong)
19:00 DINNER

Day 4. August 23.

9:00-10:00 A.R. Oganov "Novel methods in the USPEX code"
10:00-11:00 G.R. Qian "Variable-cell NEB and transition path sampling methods"
11:00-11:15 Tea break
11:15-11:45 Z. Allahyari "Searching through Mendeleevian space"
11:45-12:00 P.E. Dolgirev "Artificial intelligence: new approaches"
12:00-14:00 LUNCH
14:00-16:00 TUTORIAL 5: Surfaces and nanoparticles (Qiang Zhu, Xiang-Feng Zhou, Qinggao Wang, Zahed Allahyari)
16:00-17:00 TUTORIAL 6: Evolutionary metadynamics (Artem R. Oganov)
17:00-19:00 TUTORIAL 7: Variable-cell nudged elastic band method (Guangrui Qian)
19:00 Workshop banquet

Day 5. August 24 - Excursion