Workshop "Crystal structure prediction with the USPEX code" (Guilin, August 2013)
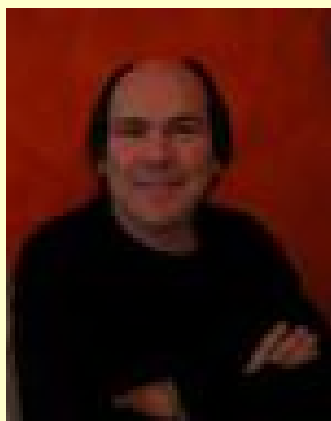
USPEX workshops

Poitiers (2011)
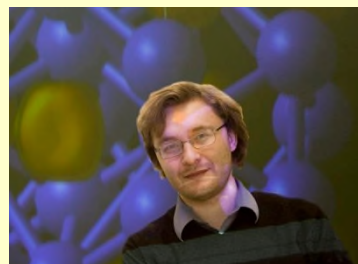FRANCE

G. Frapper

Xi'an (2011)
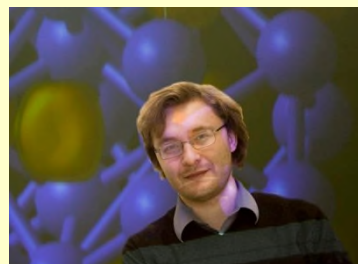CHINA

Q.F. Zeng

USPEX workshops

Lausanne (2012)
SWITZERLAND

A.O. Lyakhov

Stony Brook (2012)
USA

A.O. Lyakhov

Lyakhov's school: in memory of Andriy Lyakhov

- 03/01/2013 – passed away
- 01/2012 – became father of twin girls
- 10/2011 - Research Assistant Professor, SUNY Stony Brook.
- 24/03/2010 – married his classmate Olga.
- 2/2009 - Postdoc, SUNY Stony Brook.
- 8/2007 - Postdoc, ETH Zurich.
- 2007 - PhD in Theoretical Physics (magna cum laude), University of Basel
- 2004 - MSc. in Physics & Computer Science, Chernivtsi University
- 11/1982 – born in Chernivtsi, Ukraine

- >24 papers and reviews (including 1 in *Nature*, 1 in *Nature Chemistry*, 4 in *PNAS*, 1 in *PRL* and 1 in *Acc.Chem.Res.*), 1 book chapter, 1 patent application.
- In 2007-2013 – main programmer of USPEX

Andriy Lyakhov
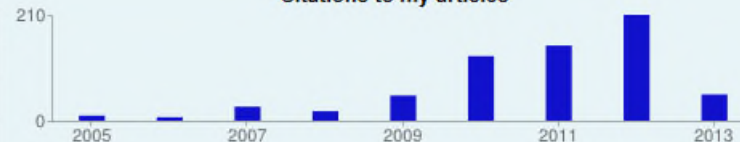Research Assistant Professor, Stony Brook University
Computational material science
Verified email at stonybrook.edu

Citation indices	All	Since 2008
Citations	659	612
h-index	15	15
i10-index	17	16

Citations to my articles

Future that could be…

Brilliant scientist, he became Res. Asst. Prof. at the age of 28. Future was to be bright.

Future that could be...

He has helped to create the tradition of USPEX workshops.
These workshops are now named Lyakhov schools.
Next Lyakhov schools to be held in 2013 – Guilin, China and Puebla, Mexico.

Future that could be…

MERRY Christmas!

25/12/2012 – one week before the tragedy.
Around 10/01/2013 planned to apply for Green Card.
Death on 03/01/2013 was sudden, without illness.
Cause of sudden death - heart infection.

# We will remember him with admiration and love

Ahmad Haghi
January 6

امروز ذهنم کلا مشغول تختی بود،

بگذریم،

صبحی وقتی جی میلم رو باز کردم، منتظر بودم اینباکس پر از ایمیل
باشه، اخه چند ماهی میشد که عضو گروه کاربران نرم افزار اسیکس
شدم و هر روز تازه واردهایی با سلیقه ها و ملیتهای مختلف در باره
چگونگی بکارگیری نرمافزار سوال می پرسند و و یه نفری به نام"اندری
لیاخوف" با دقت و حوصله به همگی شون جواب می داد، و یه نسخه از
این پرسش و پاسخ برای من ایمیل میشد، عجب کار خسته کننده ای!!
من فکر کردم این آقا باید کارمند یا مسئول پاسخگویی باشه!!!
این ها رو گفتم تا بگم امروز تنها یه ایمیل داشتم و اون این بود:
In the early morning of January 3, 2013, Andriy Lyakhov
.suddenly passed away

حالا جالب اینجاست که این جناب مرحوم، در حالی که تنها سی سال
سن داشتن و استاد زمین شناسی در دانشگاه ایالتی استونی بروک
بودند- و هیچ اجباری برای پاسخ دادن به اون همه ایمیلی که منو هم
کلافه کرده بود نداشتند!!!
در پیام های تسلیتی که ارسال شده بود همگی به اینکه مرحوم خیلی
کمک کارشون بوده، اعتراف کرده بودن!
به گفته رییس مجموعه اسیکس، آقای
Artem R. Oganov
این مرحوموقتی که تنها 16 سال داشت، نخستین مقاله علمی اش رو
به چاپ رسونده بود!! فکرشو بکن، شانزده سال!!!
امروز هفدهم دی ماه و سالگرد جهان پهلوان تختی بود!
!and It was too early for pah-lavan Andriy Lyakhov

Scientific community was shocked by his sudden death.

I have received >100 letters of condolences, from friends and foes, from people who knew Andriy well, and from those who never met him, but knew his work.

We will remember him with admiration and love
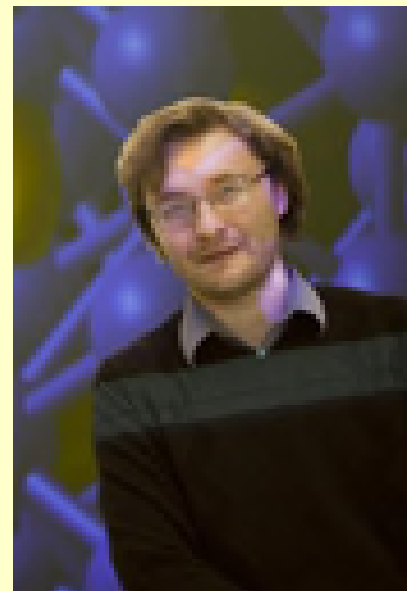
USPEX workshops are FUN!

5th USPEX workshop (Guilin, 2013)

Professor Chaohao Hu (Guilin)

6th USPEX workshop?
In Poitiers (France) in 2014.

7th USPEX workshop?
Maybe in Nalchik (Russia) in 2014.

Basic Facts on USPEX

- The most popular structure prediction code in the world (>1400 users).
- The largest (98 MB) and the most versatile code in this field. Many of its capabilities are unique.
- Interfaced with most popular ab initio codes (VASP, SIESTA, Q.Espresso, …)
- The fastest and the most reliable structure prediction code today.
- Took effort of ~40 man-years, with >$10 million of attracted funding.
- THE CODE IS FREE, but you have to agree to certain conditions of fair use **(register now!)**.

- Every year ~2 USPEX workshops.
- USPEX mailing list **(join it!)**. USPEX Forum **(use it!).**
- USPEX Facebook page **(join it!)**.
- USPEX QQ group (group number 326701679 – **join it!**)
- 4-5 visiting scholars every year in the Oganov laboratory.

*"USPEX" ("oo-spe-kh") means "success" in Russian

Features of the USPEX code:

Algorithm:

- Evolutionary optimization (USPEX algrorithm). Options to use random sampling, minima-hopping-like, particle-swarm optimization, metadynamics-like algorithms.
- Initialization using fully random, symmetric random structures, or user-fed structures (seeding).
- Fingerprint niching technique, local order parameter (ARO&Valle, 2009). Graph theory and Brown's model for analyzing topology. New variation operators (Lyakhov & ARO, 2010).

Types of runs:

- Global optimization of either the energy or properties (density, hardness, band gap, etc.)
- Fixed-cell or variable-cell, fixed-composition or variable-composition runs are possible.
- For molecular crystals, can operate with ready-made molecules.

Software aspects:

- Interfaced with VASP, SIESTA, CP2k, QuantumEspresso, DMACRYS, GULP.
- Excellent parallel scaling on up to $>10^4$ CPUs.

Analysis:

- Automatic detection of space groups.
- Benefits from powerful analysis and visualization code STM4.

Distribution:

- **USPEX code is freely available at: http://uspex.stonybrook.edu**
- Code distributed with a 50-page manual and ~21 tutorials/tests.
- USPEX Users and Developers Community (>1400 people)

Statistics

- \>1400 users from 69 countries.

- 352 USA
- 338 China
- 90 India
- 41 U.K.
- 37 S. Korea
- 45 Russia
- 37 Germany
- 32 Japan
- 30 France
- 26 Australia
- 24 Spain
- 19 Turkey
- 19 Iran
- 18 Brazil
- 18 Poland
- 17 Italy

People behind USPEX
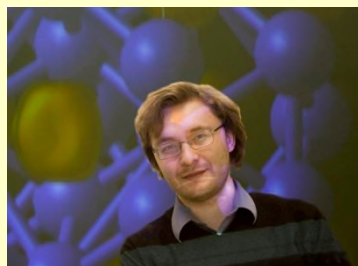
A.O. Lyakhov

Q. Zhu

H.T. Stokes

S.E. Boulfelfel

C.W. Glass

Miguel Salvado
& Pilar Pertierra

G.R. Qian

Q.F. Zeng

M. Valle

A.R. Oganov

Funding of USPEX

- Industrial partners: Intel, Samsung, Toyota, Fujitsu.

Announcements: Participants shaping the workshop

1. Talks by participants – please talk to us (CHH and ARO) if you would like to present your work in a talk.

2. Everybody is welcome to present posters.

3. Talk to me (ARO) if you want to study a particular problem during this workshop.

4. We have special prizes for this!

Announcement:

Multiple PhD and postdoc positions are available in 3 USPEX laboratories, for up to 3-5 years.

3 laboratories: US (Stony Brook), Russia (Moscow), China (Xi'an).

If interested, please contact me: artem.oganov@stonybrook.edu.