

**ES'PA 2015**

22-24 june, 2015 Poitiers (France)

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**9th USPEX workshop**

25-30 june, 2015 Poitiers (France)

**D1.** Thursday 25 june / 2-6 pm

- 14:00-14:30 Welcome – A.R. Oganov & G. Frapper  
 14:30-16:00 A.R. Oganov "Crystal structure prediction and the USPEX code"  
 16:00 -16:30 Coffee break  
 16:30-18:00 *TUTORIALS* : Installation party / First steps with USPEX  
 19:00-21:00 Dinner  
 21:00-23:00 Open lab: VASP, GULP (? For clusters), QE, FHI-AIM... (S. de Gironcoli, etc)

**D2.** Friday 26 june / 9 am-6 pm

- 9:00-10:30 A.R. Oganov "optimization of physical properties"  
 10:30-11:00 coffee break + Poster session  
 11:00-12:00 C. Gatti « Solving chemistry puzzles in molecules and crystals through  
 electron and electron spin density analyses »  
*Photo group*  
 12:00-14:00 Lunch  
 14:00-18:00 *TUTORIALS*:  
 - tutorial on data analysis (X, Y)  
 - prediction of high-pressure phases (A.R. Oganov, X)  
 18:00-19:30 Apéro-Rock!  
 19:30-21:00 Dinner

**D3.** Saturday 27 june / 9 am-6 pm

- 9:00-10:00 Q. Zhu "Prediction of the structure of molecular crystals"  
 10:00-10:30 2-3 TALKS OF THE PARTICIPANTS flash presentation (G. Frapper)  
 10:30-11:00 coffee break + Poster session  
 11:00-12:00 Q. Zhu "Variable-composition evolutionary structure prediction"  
 12:00-14:00 Lunch  
 14:00-18:00 *TUTORIALS*:  
 molecular crystals (Q. Zhu, X)  
 variable-composition structure predictions (X)

*dinner "en ville" off - free*

**D4.** Sunday 28 june / social event. Starting 11 am

Loire river pique-nique, Fontevraud, wine tasting / Gala Dinner

***Open!***

**D5.** Monday 29 june / 9 am-6 pm

9:00-10:00 P. Johari "Theory and simulations of low-dimensional systems"

10:00-10:30 2-3 TALKS OF THE PARTICIPANTS flash presentation (G. Frapper)

10:30-11:00 coffee break + Poster session

11:00-12:00 Q. Zhu "Evolutionary structure prediction for nanoparticles and surfaces"

12:00-14:00 *Lunch*

14:00-15:00 Round table - your research using USPEX

15:00-18:00 *TUTORIALS*: nanoparticles, 2D crystals and surfaces (Q. Zhu, G. Frapper, X)

19:00-21:00 Dinner

21:00-23:00 Open lab: your research using USPEX, first steps (trainers)

**D6.** Tuesday 30 june / 9 am-4 pm

9:00-10:30 A.R. Oganov "Evolutionary metadynamics"

10:30-11:00 coffee break + Poster session

11:00-12:00 *TUTORIALS*: evolutionary metadynamics (A.R. Oganov, X)

12:00-14:00 *Lunch*

14:00-16:00 *TUTORIALS*: evolutionary metadynamics (A.R. Oganov, X)

16:00 end – A.R. Oganov & the 9<sup>th</sup> USPEX team

**Lecturers / trainers** : A.R. Oganov, C. Gatti, P. Johari , S. de Gironcoli, Q. Zhu , B. Huang, S. Yu, Weicong et G. Frapper (to be complete)

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*Tentative plan*

	Monday 22 June	Tuesday 23 June	Wednesday 24 June
8h30		Coffee welcome (Conference center)	Coffee welcome (Conference center)
9:00-10:30		<i>S. de Gironcoli</i> Quantum Espresso code	<i>S. de Gironcoli</i> DFT vs others approaches
10:30-10:45		Coffee break	Coffee break
10:45-11:30		Sergey Levchenko FHI-aim	<i>G. Frapper</i> From bulk to surface
11:30-12:15		<i>X</i> VASP code	<i>Hands-on lab</i> (cont'd) Bulk materials
12:30-14:00		LUNCH	LUNCH
14:00	14:00 Welcome	<i>Hands-on lab</i>	<i>Hands-on lab</i>
	15:00 <i>V. Mauchamp</i> Electronic wave functions in periodic systems	Starting with VASP/ QE / FHI-aim  Bulk materials	Basics modeling of surfaces & molecules
16:30-17:00	Coffee	Coffee	Coffee
17:00-18:30	<i>XX</i> ABC on DFT	<i>Hands-on lab</i> Bulk materials (cont'd)	<i>Hands-on lab</i> (cont'd)
18:30- 21:00	Pause + diner	Pause + diner	end
21:00	<i>Open lab</i> <i>B. Huang, S. Yu, C. Mastail</i> Linux for beginners / installation party (on your laptop)	<i>Open lab</i> <i>B. Huang, S. Yu, C. Mastail</i> Practice on your bulk materials (on your laptop)	

**Lecturers / trainers** : S. de Gironcoli, V. Mauchamp, C. Mastail, , B. Huang, S. Yu, C. Dong et G. Frapper (to be completed)