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# Workshop on Crystal Structure Prediction: Exploring the Mendeleev Table as a Palette to Design New Materials | (smr 3267)

## Monday 14 January 2019

### **DAY 1: Morning session Chairperson: Sandro Scandolo - Kastler Lecture Hall (AGH)** **(08:30-14:30)**

time	title	presenter
08:30	REGISTRATION OF VISITS / ADMINISTRATIVE ISSUES, and welcome coffee from 10:00	
10:20	Opening remarks	
10:30	Computational Materials Discovery using USPEX Method/Code	OGANOV, Artem
11:10	Random search - challenges and new directions	PICKARD, Chris
11:50	The Importance of the Mendeleev (Periodic) Number in Crystal Structure Prediction - a Data-Centric Approach	VILLARS, Pierre
12:30	Lunch break	

### **DAY 1: Afternoon session Chairperson: Erio Tosatti - Adriatico Guest House - Kastler Lecture Hall (14:30-17:30)**

time	title	presenter
14:30	Beyond SiO <sub>2</sub> : New tetrahedral and octahedral structures in IV-VI compounds	MARTONAK, Roman
15:10	Exploring the potential energy surface of synthesizable and non-synthesizable clusters with the Minima Hopping method	GOEDECKER, Stefan
15:50	Coffee break	
16:20	Short presentations of posters	

### **DAY 1: Poster Session - Kastler Lecture Hall (AGH) (17:30-20:00)**

time	title	presenter
17:30	Poster session outside the Kastler Lecture Hall	