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

Wednesday 16 January 2019

DAY 3: Morning Session Chairperson: Stefano de Gironcoli - Adriatico Guest House - Kastler Lecture Hall (09:00-14:30)

time	title	presenter
09:00	Potential of Neural Networks for Crystal Structure Prediction of Molecular Crystals	KUCUKBENLI, Emine
09:40	Self-consistent harmonic approximation: an efficient tool to evaluate the phase diagram with thermal and quantum nuclear fluctuations in crystals	MONACELLI, Lorenzo
10:10	Coffee break	
10:50	Computational search for supermaterials with optimal properties	KVASHNIN, Alexander
11:30	Density functional studies on compositional mixing of metal-halide perovskites	HONG, Ki-Ha
11:50	Random Search for Interface Structure Prediction - Computational Discovery Going Beyond Crystals	SCHUSTERITSCH, Georg
12:10	Searching for mixtures of planetary ices	NADEN ROBINSON, Victor
12:30	Lunch break	

DAY 3: Afternoon session, Chairperson: Stefano Baroni - Adriatico Guest House - Kastler Lecture Hall (14:30-16:30)

time	title	presenter
14:30	■Coevolutionary search for optimal materials in the space of all possible compounds	ALLAHYARI, Zahed
15:10	Entropy as a tool for crystal discovery	PIAGGI, Pablo
15:50	Coffee break	