GreenALM hands-on tutorial 2021

Preliminary program (status Aug. 9, 2021)

Start Monday, 11 October 2021
End Thursday, 14 October 2021

Time	Topic	Speaker
	Monday, 11 October 2021	
14:00	Welcome+General introduction	J. Spitaler, O. Peil. A. Ruban
14:30	Basics of DFT	C. Draxl
15:30	Introduction to electronic structure calculations with GreenALM: Green's function DFT; Simple metals ... SCF cycle, convergence tests, equation of state, band structure, Fermi surface	A. Ruban
16:00	*Coffee break*	
16:20	Hands-on session I	
18:00	*END*	
	Tuesday, 12 October 2021	
09:00	Green's function DFT for alloys	J. Staunton
10:00	Introduction to basic alloy calculations with GreenALM: CPA, scf cycle, formation energy	O. Peil
10:30	*Coffee break*	
10:50	Hands-on session II	
12:30	*Lunch break*	
14:00	Structural transitions	S.Simak
15:00	Introduction to calculations of alloy properties (phase equilibria, segregation, etc.) with GreenALM	A. Ruban
15:30	*Coffee break*	
15:50	Hands-on session III	
17:30	*END*	
	Wednesday, 13 October 2021	
09:00	Thermodynamic and mechanical properties at finite temperatures	P. Korzhavyi
10:00	Introduction to phase stability with GreenALM	J. Spitaler
10:30	*Coffee break*	
10:50	Hands-on session IV	
12:30	*Lunch*	
14:00	Defects in metals and alloys at finite temperatures from DFT	B. Grabowski
15:00	Introduction to alloy thermodynamics with GreenALM	A. Ruban
15:30	*Coffee break*	
15:50	Hands-on session V	
17:30	*END*	
	Thursday, 14 October 2021	
09:00	Multi-scale simulation of mechanical properties and solid solution strengthening (SSS)	F. Maresca
10:00	Introduction to SSS workflow based on GreenALM	F. Moitzi
10:30	*Coffee break*	
10:50	Hands-on session VI	
12:30	*Lunch break*	
14:00	Reassessment of CALPHAD data bases combining experiment and DFT	*L. Romaner*
14:45	Accelerated alloy design based on machine learning and DFT.	O. Peil/J. Spitaler
15:30	*Coffee break*	
15:50	Hands-on session VII	
17:30	*Final remarks*	J. Spitaler, O. Peil. A. Ruban
18:00	*END OF TUTORIAL*	