

Virtual Psi-k GreenALM hands-on tutorial 2021

Program



Date	Time	Topic	Speaker
Mon. 11 Oct. '21	14:00	Welcome and general introduction	O. Peil, A. Ruban, J. Spitaler
	14:30	Basics of Density Functional Theory	C. Draxl
	15:30	Introduction to the machinery of GreenALM	O. Peil
	16:00	<i>Coffee break</i>	
	16:20	Hands-on session I: Electronic structure and EOS	Tutors/Breakout sessions
	18:00	<i>END</i>	
Tue. 12 Oct. 2021	09:00	Green's function DFT for alloys	J. Staunton
	10:00	Introduction to calculations of random alloys with GreenALM	O. Peil
	10:30	<i>Coffee break</i>	
	10:50	Hands-on session II: Electronic structure of random alloys using CPA	Tutors/Breakout sessions
	12:30	<i>Lunch break</i>	
	14:00	Structural transitions	S.Simak
	15:00	Introduction to calculation of alloy properties with GreenALM	A. Ruban
	15:30	<i>Coffee break</i>	
	15:50	Hands-on session III: Alloy formation energies and phase equilibria	Tutors/Breakout sessions
	17:30	<i>END</i>	
Wed. 13 Oct. 2021	09:00	Thermodynamic and mechanical properties at finite temperatures	P. Korzhavyi
	10:00	Introduction to magnetic calculations	A. Ruban
	10:30	<i>Coffee break</i>	
	10:50	Hands-on session IV: Magnetic fluctuations with GreenALM	Tutors/Breakout sessions
	12:30	<i>Lunch</i>	
	14:00	Defects in metals and alloys at finite temperatures from DFT	B. Grabowski
	15:00	Introduction to thermal properties with GreenALM	J. Spitaler
	15:30	<i>Coffee break</i>	
	15:50	Hands-on session V: Thermo-mechanical properties	Tutors/Breakout sessions
	17:30	<i>END</i>	
Thu. 14 Oct. 2021	09:00	Ab-initio informed thermokinetic modeling of metallic alloys	L. Romaner
	09:45	Accelerated alloy design based on machine learning and DFT.	O. Peil, J. Spitaler
	10:30	<i>Coffee break</i>	
	11:00	Multi-scale simulation of mechanical properties and solid solution strengthening (SSS)	F. Maresca
	12:00	<i>Lunch</i>	
	13:30	Introduction to SSS workflow based on GreenALM	F. Moitzi
	14:00	Hands-on VI: SSS with GreenALM	Tutors/Breakout sessions
	15:30	Concluding remarks	J. Spitaler
	15:45	<i>END OF TUTORIAL</i>	

