OAK RIDGE National Laboratory

AGENDA

MANAGED BY UT-BATTELLE FOR THE US DEPARTMENT OF ENERGY

Virtual- workshop on Magnetic Structures Determination
Sept 28 – Oct 2, 2020

Monday, September 28, 2020

Time (EDT = UTC-4)	**Event**
9:30 - 9:45	Welcome and Introductory remarks; Agenda overview *Bryan Chakoumakos & Clarina dela Cruz*
9:45 - 10:45	Experimental aspects of magnetic structure determination *Speaker: William Ratcliff / Moderator: Clarina dela Cruz*
10:45 - 12:00	Symmetry based modeling and description of magnetic structures: Magnetic space groups *Speaker:* J. *Manuel Perez-Mato / Moderator: Bryan Chakoumakos*
12:00 - 12:15	Break
12:15 - 13:30	Hands-on demonstration of Bilbao Crystallographic Server: MAXMAGN, k-SUBGROUPSMAG, MVISUALIZE, MAGDATA *Speaker:* J. *Manuel Perez-Mato / Moderator: Bryan Chakoumakos*
13:30-14:30	Introduction to the FullProf Suite. Options to define the magnetic structure models in FullProf *Speaker: Juan Rodriguez-Carvajal / Moderator: Ovidiu Garlea*
14:30 - 14:45	Break
14:45-16:15	Example of FullProf refinement of commensurate structure from constant wavelength powder diffraction data (Magnetic SG approach) - Ex FP 1 *Speaker: Stuart Calder/ Moderator: Keith Taddei*

OAK RIDGE National Laboratory

AGENDA

MANAGED BY UT-BATTELLE FOR THE US DEPARTMENT OF ENERGY

Tuesday, September 29, 2020

Time (EDT = UTC-4)	**Event**
9:30 -11:00	Example of FullProf refinement of commensurate structure from TOF powder diffraction data (Magnetic SG approach) - Ex FP 2 *Speaker: Ovidiu Garlea / Moderator: Stuart Calder*
11:00-11:15	Break
11:15 - 12:45	Example of FullProf refinement of commensurate structure from single-crystal data (Magnetic SG approach) - Ex FP 3 *Speaker: Huibo Cao / Moderator: Clarina dela Cruz*
12:45 - 13:00	Break
13:00 - 14:00	Representation Theory in Magnetic Structure Analysis *Speaker: Juan Rodriguez-Carvajal / Moderator: Ovidiu Garlea*
14:00 - 15:00	Demonstration of SARAh Representational Analysis programs *Speaker: Andrew Wills / Moderator: Keith Taddei*
15:00 - 15:15	Break
15:15-16:15	Introduction to ISOTROPY software *Speaker: Branton Campbell / Moderator: Bryan Chakoumakos*

OAK RIDGE National Laboratory

AGENDA

MANAGED BY UT-BATTELLE FOR THE US DEPARTMENT OF ENERGY

Wednesday, September 30, 2020

Time (EDT = UTC-4)	Event
9:30 – 10:30	How to report magnetic structures in publications & prepare mcif files *Speaker: J. Manuel Perez-Mato / Moderator: Ovidiu Garlea*
10:30 - 10:45	Break
10:45 – 12:15	Example of Fullprof refinement of commensurate structure from powder diffraction data (basis vectors of Irreducible representations) -Ex FP 4 *Speaker: Keith Taddei / Moderator: Stuart Calder*
12:15 - 12:30	Break
12:30 - 14:00	Example of Fullprof refinement of incommensurate (IC) structure from powder data (basis vectors of Irreducible representations) - Ex FP 5 *Speaker: Stuart Calder / Moderator: Clarina dela Cruz*
14:00-14:15	Break
14:15-15:45	Example of Fullprof refinement of incommensurate structure from single crystal data (basis vectors of Irreducible representations) - Ex FP 6 *Speaker: Huibo Cao / Moderator: Yan Wu*

OAK RIDGE National Laboratory

AGENDA

MANAGED BY UT-BATTELLE FOR THE US DEPARTMENT OF ENERGY

Thursday, October 1, 2020

Time (EDT = UTC-4)	**Event**
9:30 -10:30	QMI at ORNL: Instrumentation and Science opportunities? *Speaker: Clarina dela Cruz / Moderator: Ovi Garlea*
10:30-11:30	Symmetry of incommensurate magnetic structures: magnetic superspace groups *Speaker: Branton Campbell / Moderator: Bryan Chakoumakos*
11:30-11:45	Break
11:45-13:15	Example of FullProf refinement of incommensurate structure from powder data (superspace group approach) - Ex FP7 *Speaker: Ovidiu Garlea / Moderator: Stuart Calder*
13:15-13:30	Break
13:30-14:30	Introduction to the GSAS2 *Speaker: Brian H. Toby/ Moderator: Efrain E. Rodriguez*
14:30 -16:00	Example of GSAS2 refinement of commensurate structure from TOF powder diffraction data - Ex_GSAS *Speaker: Keith Taddei / Moderator: Huibo Cao*

OAK RIDGE National Laboratory

AGENDA

MANAGED BY UT-BATTELLE FOR THE US DEPARTMENT OF ENERGY

Friday, October 2, 2020

Time (EDT = UTC-4)	**Event**
9:30 -10:00	Introduction to the JANA *Speaker: Vaclav Petricek / Moderator: Xiaoping Wang*
10:00-10:15	Break
10:15-11:45	Example of JANA refinement of magnetic structure on powder diffraction data - Ex_JANA *Speaker: Margarida Henriques / Moderator: Xiaoping Wang*
11:45 - 12:00	Break
12:00 - 13:00	A hierarchy of magnetic structures based on lattice dimensionality. *Speaker: Ovidiu Garlea / Moderator: Stuart Calder*
13:00- 14:00	Past and Future workshops on magnetic structure. *Speaker: Efrain E. Rodriguez / Moderator: Bryan Chakoumakos*
13:00 – 14:00	Discussions and closing remarks. *Moderator: Ovidiu Garlea*