**Magnetic Structure Determination from Neutron Diffraction Data (MagStr), October 3-7, 2022**

Oak Ridge National Laboratory, Building 8600, Room C-156

**Monday October 3, 2022**

| Time | **Event** | **Presenter** |
| --- | --- | --- |
| 8:30 – 9:00am | Registration/Breakfast |  |
| 9:00 – 9:30am | Welcome and workshop overview |  |
| 9:30 – 10:30am | Neutron scattering as a tool for magnetic structures determination | William Ratcliffe |
| 10:30 – 10:45am | Break |  |
| 10:45 – 12:00 | Symmetry based modeling and description of Magnetic structures: Magnetic Space Groups | J. Manuel Perez-Mato |
| 12:00 – 1:00pm | Working Lunch: Overview of available software tools for magnetic structure determination/visualization | Ovi Garlea |
| 1:00 – 1:45pm | Introduction to Fullprof Suite. Options to define magnetic structure models and future software developments | J. Rodriguez-Carvajal |
| 1:45 – 2:45pm | Hands on demonstration of Bilbao Crystallographic server: MAXMAGN, MVISUALIZE, k-SUBGROUPSMAG etc | J. Manuel Perez-Mato |
| 2:45 – 3:00pm | Break |  |
| 3:00 – 3:45pm | Description of Magnetic-CIF and MAGDATA database | J. Manuel Perez-Mato |
| 3:45 – 5:30pm | Example of Fullprof refinement of commensurate structures from CW powder diffraction data [Fullprof/Bilbao Magnetic Space Groups] | Stuart Calder |
| 5:30 – 6:00pm | Student questions from the day | EVERYONE |

**Tuesday October 4, 2022**

| Time | **Event** | **Presenter** |
| --- | --- | --- |
| 8:30 – 9:00 am | Breakfast snack / Questions from previous day | Everyone |
| 9:00 – 10:30 am | Fullprof refinement of commensurate structure from TOF data (Fullprof/ magnetic space group approach) | Qiang Zhang |
| 10:30 – 10:45 am | Break |  |
| 10:45 – 12:00 pm | Fullprof refinement of single crystal data (commensurate structure with magnetic space group approach) | Huibo Cao |
| 12:00 – 1:00 pm | Working Lunch: Neutron diffractometers at ORNL | Clarina dela Cruz |
| 1:00 – 2:30 pm | Representation theory in magnetic Structure Analysis | Andrew Wills |
| 2:30 – 3:30 pm | Demonstration of SARAh Representational Analysis | Andrew Wills |
| 3:30 – 3:45pm | Break |  |
| 3:45–5:30pm | Introduction to ISOTROPY and hands-on examples | Branton Campbell |
| 5:30–6:00pm | Student questions from the day | EVERYONE |

**Wednesday October 5, 2022**

| Time | **Event** | **Presenter** |
| --- | --- | --- |
| 8:30 – 9:00 am | Breakfast snack / Questions from previous day | Everyone |
| 9:00 – 10:30 am | Fullprof refinement for commensurate and incommensurate magnetic structures from CW powder data (basis vectors/irreps) (part-1) | Stuart Calder |
| 10:30 – 10:45 am | Break |  |
| 10:45 – 12:00 | Fullprof refinement for commensurate and incommensurate magnetic structures from CW powder data (basis vectors/irreps) (part-2) | Ovi Garlea |
| 12:00 – 1:00 pm | Working Lunch: Resources, engagement and community activities for neutron scattering | Efrain Rodriguez |
| 1:00 – 2:30 pm | Fullprof refinement of single crystal data (incommensurate structure with irrep approach) | Huibo Cao |
| 2:30 – 2:45 pm | Break |  |
| 2:45 – 4:00 pm | Symmetry of incommensurate magnetic structures: magnetic superspace groups | Branton Campbell |
| 4:00 – 5:30 pm | Fullprof incommensurate structure from powder data (superspace group) | Ovi Garlea |
| 5.30 – 7.00pm | POSTER SESSION and DINNER | EVERYONE |

**Thursday October 6, 2022**

| Time | **Event** | **Presenter** |
| --- | --- | --- |
| 8:30 – 9 am | Breakfast snack / Questions from previous day | Everyone |
| 9:00 – 10:00 am | Fullprof: double-k magnetic structure from powder data (Irreps and MSG approaches) | Ovi Garlea |
| 10:00 – 10:30 am | Fullprof: double-k magnetic structure from single-crystal data | Huibo Cao |
| 10:30 – 10:45 am | Break |  |
| 10:45 – 11:30 am | How to report magnetic structures in publications and submit mcif files to MAGDATA (tutorial) | J. Manuel Perez-Mato |
| 11:30 – 12:00 am | Prepare a mcif files from a publication on your own (groups working independently on examples of published structures)-part1 | Everyone |
| 12:00 – 1:00 pm | Working Lunch: Sample environments | Stuart Calder |
| 1:00 – 2:00 pm | Prepare a mcif files from a publication on your own (groups working independently on examples of published structures)- part2 | Everyone |
| 2:00 – 3:00 pm | Introduction to GSAS-II/ Magnetic structure in GSAS-II | Brian Toby |
| 3:00 - 3:15 pm | Break |  |
| 3:15 – 4:45pm | Example of GSAS-II refinement of magnetic structure from CW powder data | Keith Taddei |
| 4:45 – 6:00 pm | Example of GSAS-II refinement of magnetic structure from TOF data | Qiang Zhang |
| 6:00–6:30pm | Student questions from the day | EVERYONE |

**Friday October 7, 2022**

| Time | **Event** | **Presenter** |
| --- | --- | --- |
| 8:30 – 9am | Breakfast snack / Questions from previous day | Everyone |
| 9:00 – 10:00am | Introduction to Jana | Vaclav Petricek |
| 10:00 – 10:30am | Break |  |
| 10:30 – 12:00 | Example of Jana refinement of magnetic structure on powder diffraction data | Margarida Henriques |
| 12:00 – 1:00 pm | Working Lunch: Writing proposals for beamtime | Clarina Dela Cruz |
| 1:00 – 2:30 pm | Example of Jana refinement of magnetic structure on single-crystal data | Zach Morgan/ Feng Ye |
| 2:30-2:45 pm | Break |  |
| 2:45-4:30 pm | Bring your own magnetic structure problems to discuss. Prepare your own mcif that is not in MAGNDATA | Everyone |
| 4:30-5:00pm | Discussion/ Closing Remarks/ Feedback | Everyone |
| 5:00-6:00pm | Tour of HFIR/SNS/Graphite reactor | Optional |