

## Tutorial on modern modeling methods in neutron spectroscopy Spallation Neutron Source - Oak Ridge National Laboratory Building 8600, C-156

**April 15<sup>th</sup> -17<sup>th</sup> 2019**

<b>Monday, April 15, 2019</b>			
<b>Time</b>	<b>Event</b>	<b>Lead</b>	<b>Place</b>
8:00-9:00am	Registration		8600, Atrium
9:00-9:15am	Welcome and Introduction	<i>Mark Lumsden, Spectroscopy Group Leader, NSD</i>	8600, C156
9:15 AM – 9:30am	Overview of the ICEMAN project	<i>Timmy Ramirez-Cuesta, ORNL</i>	8600, C156
9:30 AM – 10:30 am	First-principles materials simulation/Introduction to DFT	<i>Keith Refson, Royal Holloway, U.K.</i>	8600, C156
10:30 AM – 11:00 am	Coffee Break		8600, C150
11:00- 12:30pm	First-principles materials simulation/Introduction to DFT (cont'd)	<i>Keith Refson, Royal Holloway, U.K.</i>	8600, C156
12:30-2:00pm	Working Lunch: “Software Installation”,	<i>Timmy Ramirez-Cuesta, ORNL</i>	8600, C156
2:00-3:00pm	Introduction to CASTEP	<i>Keith Refson, Royal Holloway, U.K.</i>	8600, C156
3:00-3:30pm	Coffee Break		8600, C150
3:30-5:30pm	CASTEP practical	<i>Keith Refson, Royal Holloway, U.K., YQ Cheng, ORNL &amp; Timmy Ramirez-Cuesta, ORNL</i>	8600, C156
5:30pm	Adjourn		

**Contact Person:** Sharon Porter (865)576-5251, email: [portersa@ornl.gov](mailto:portersa@ornl.gov)

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<b>Tuesday, April 16, 2019</b>			
<b>Time</b>	<b>Event</b>	<b>Lead</b>	<b>Place</b>
9:00-10:30am	Introduction to CP2K/Molecular dynamics	<i>Greg Schenter/Shawn Kathmann, PNNL</i>	8600, C156
10:30 – 11:00 am	Coffee Break		8600, C150
11:00- 12:30pm	CP2K practical	<i>Greg Schenter/Shawn Kathmann, PNNL</i>	8600, C156
12:30-2:00pm	Working Lunch: “TBD”		8600, C156
2:00-3:00pm	Introduction to QENS and its applications	<i>Eugene Mamontov, ORNL</i>	8600, C156
3:00-3:30pm	Coffee Break		8600, C150
3:30-5:30pm	Classical MD and LiquidLib	<i>Yang Zhang, UIUC</i>	8600, C156
5:30-8:00pm	Poster session and on-site dinner, SNS lobby		8600, Atrim
8:00pm	Adjourn		

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<b>Wednesday, April 17, 2019</b>			
<b>Time</b>	<b>Event</b>	<b>Lead</b>	<b>Place</b>
9:00 – 10:30 am	Advanced QENS data analysis with QClimax	<i>Timmy Ramirez-Cuesta, ORNL</i>	8600, C156
10:30– 11:00 am	Coffee Break		8600, C150
11:00- 12:30pm	QClimax practical	<i>Timmy Ramirez-Cuesta, ORNL</i>	8600, C156
12:30-2:00pm	Working Lunch: TBD		8600, C156
2:00-3:00pm	INS simulation with OClimax	<i>YQ Cheng, ORNL</i>	8600, C156
3:00-4:00pm	OClimax practical	<i>YQ Cheng, ORNL</i>	8600, C156
4:00pm	Adjourn		

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