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Virtual Institute: New States of Matter and Their Excitations

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Neutron Sciences Directorate

CRADA FINAL REPORT
Virtual Institute: New States of Matter and Their Excitations

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September 30, 2018

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Abstract
This is the final report on the CRADA "Virtual Institute: New States of Matter and Their Excitations" executed between the Helmholtz Zentrum Berlin and the Oak Ridge National Laboratory.

Statement of Objectives
This CRADA enabled participation by ORNL staff in the "Helmholtz Virtual Institute (No. VH-VI-521); New states of matter and their excitations." This project was funded by a grant to the Helmholtz Zentrum Berlin (HZB) by the Helmholtz Gemeinschaft (HGF). The project provided travel money for ORNL personnel to participate in meetings of the virtual institute in order to encourage collaborative research. No funding was exchanged between the participants, except that HZB paid travel costs for VI activities when necessary.

In addition to personnel from HZB and ORNL, the virtual institute (VI) included numerous faculty members at German Universities and institutes, notably including the Max Planck Institute for the Physics of Complex Systems (MPIPKS) in Dresden, and other international participants, including from the UK (Oxford and Cambridge Universities), and the USA (Princeton University and California Institute of Technology).

The deliverables included ORNL participation in VI meetings and conferences, VI personnel participating in ORNL workshops, and joint papers from collaborations established through the virtual institute.

Benefits to the Funding DOE Office's Mission
The ORNL participants' programs are sponsored by the Office of Science, Basic Energy Sciences, Division of Scientific User Facilities. This CRADA enabled collaborations with world leading researchers in quantum materials, especially theorists, and resulted in several high-profile publications that used ORNL's neutron scattering facilities.

Technical Discussion of the Work Performed by All Parties
The participants engaged in theoretical and experimental work on new states of matter and their excitations. The experimental work emphasized the use of inelastic neutron scattering to characterize such excitations, and the theoretical work emphasized the interpretation of these experiments. Other techniques were used as well.

Although it was anticipated that the HGF would fund the VI at HZB for 5 years, a decision was taken to halt the funding early. As a result, formal participation by ORNL personnel in official VI meetings in Germany was limited to three meetings in Berlin, Gottingen, and Dresden, the last ending early in FY 2015. Despite this the meetings seeded several successful collaborations, notably between ORNL and the MPIKPS as well as Princeton, which subsequently led to important collaborative science and several high-profile scientific publications arising from work carried out after the termination of VI funding. This has contributed significantly to the success of the scientific programs at these Institutions.

The collaborations continue to pay dividends, and a list of the joint publications to date with collaborations that originated from the VI appears below:

- S. Isakov, **R.** Moessner, D. L. Sondhi, D. A. Tennant, *Analytical theory of the proton correlations in Ice Ih*, Phys. Rev. B 91 245152 (2015).
- A. Banerjee, C. A. Bridges, J.-Q. Yan, A.A. Aczel, L. Li, M. B. Stone, G,. E. Granroth, M.D. Lumsden, Y. Yiu, J. Knolle, D. L. Kovrizhin, S. Battacharjee, R. Moessner, D.A. Tennant, D.G.

Mandrus, S.E. Nagler, *Proximate Kitaev Quantum Spin Liquid Behaviour in α-$RuCl_3$*, arXiv:1504.08037, Nature Materials **15**, 733, DOI:10.1038/NMAT4604 (2016).

- Arnab Banerjee, Jiaqiang Yan, Johannes Knolle, Craig A. Bridges, Matthew B. Stone, Mark D. Lumsden, David G. Mandrus, David A. Tennant, Roderich Moessner, Stephen E. Nagler, *Neutron scattering in the proximate quantum spin liquid α-$RuCl_3$*, arXiv:1609.0013, SCIENCE **356**, 1055 (2017), DOI: 10.1126/science.aah6015.
- A. Banerjee, P. Lampen-Kelley, J. Knolle, C. Balz, A.A. Aczel, B. Winn, Y. Liu, D. Pajerowski, J-Q. Yan, C.A. Bridges, A. Savici, B. C. Chakoumakos, M. D. Lumsden, D.A. Tennant, R. Moessner, D.G. Mandrus, and S.E. Nagler, *Excitations in the field-induced quantum spin liquid state of α-$RuCl_3$*, , arXiv:1706.07003, NPJ Quantum Materials **3**,: 8 (2018), doi:10.1038/s41535-018-0079-2.
- R. Hentrich, A. U. B. Wolter, X. Zotos, W. Brenig, D. Nowak, A. Isaeva, T. Doert, A. Banerjee, P. Lampen-Kelley, D. G. Mandrus, S. E. Nagler, J. Sears, Y.-J. Kim, B. Buchner, C. Hess, *Unusual phonon heat transport in α-$RuCl_3$: Strong spin-phonon scattering and field-induced spin gap* arXiv:1703.08623, Phys. Rev. Lett. **120**, 117204 (2018).
- G. Bastien, G. Garbarino, R. Yadav, F. J. Martinez-Casado, R. Beltrán Rodríguez, Q. Stahl, M. Kusch, S. P. Limandri, R. Ray, P. Lampen-Kelley, D. G. Mandrus, S. E. Nagler, M. Roslova, A. Isaeva, T. Doert, L. Hozoi, A. U. B. Wolter, B. Büchner, J. Geck, J. van den Brink, *Pressure-induced dimerization and valence bond crystal formation in the Kitaev-Heisenberg magnet α-$RuCl_3$*, arXiv:1802.09861, Phys. Rev. B **97**, 241108 (2018).
- P. Lampen-Kelley, S. Rachel, J. Reuther, J.-Q. Yan, A. Banerjee, C.A. Bridges, H.B. Cao, S.E. Nagler, D. Mandrus, *Anisotropic susceptibilities in the honeycomb Kitaev system α-$RuCl_3$*, arXiv:1803.04871, accepted as a Rapid Communication in PRB (2018).
- P. Lampen-Kelley, L. Janssen, E. C. Andrade, S. Rachel, J.-Q Yan, C. Balz, D. Mandrus, S. Nagler, and M. Vojta, *Field-induced intermediate phase in α-$RuCl_3$*: Non-coplanar order, phase diagram, and proximate spin liquid, arXiv:1807.06192, Nature Communications, under review (2018).
- J.P. Morris, D.J.P. Morris, K. Siemensmeyer, J.-U. Hoffmann, B. Klemke, I. Glavatskyi, K. Seiffert, D.A. Tennant, S.V. Isakov, S. Sondhi, R. Moessner, *Neutron study of the topological flux model of hydrogen ions in water ice* SCIENCE, under review (2018).

Subject Inventions

None – not applicable

Commercialization Possibilities

None known at this time

Plans for Future Collaboration

It is expected that going forward ORNL personnel will continue informal collaborations with leading researchers who were affiliated with the Virtual Institute.

Conclusions

The CRADA "Virtual Institute: New States of Matter and Their Excitations" contributed to the initiation of several collaborations between ORNL based researchers and world-leading researchers based elsewhere, and led to several high-profile publications that utilized data obtained at ORNL neutron scattering facilities.