

Project Title:**Computational Studies of muon location, electronic structure and hyperfine interactions in high Tc Superconductors, Organic and Organometallic System****Name:**

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<p>1. Background</p> <p>Muon Spin Rotation (μSR) technique is an excellent method to study the magnetic properties and electronic structures of materials. It can be applied to diverse class of materials such as high Tc superconductors and organic magnets. There is a need for a close collaboration between experimental efforts and computational studies so that the underlying science of the materials of interest could be unraveled. One of the main objectives for the computational studies is to study the stopping sites for muon and muonium. Knowledge about the muon and muonium stopping sites could pave a way to enhance our understanding about the materials. The μSR experiments have been conducted at the RIKEN-RAL μSR facility in the United Kingdom and the Paul Scherer Institute in Switzerland, while the computational studies were carried out using the excellent supercomputing facilities provided by the Advanced Center for Computing and Communication at RIKEN.</p> <p>We are currently working on the following projects that are computational in nature which involve muon in different host materials. The host materials are:</p> <p>i) Organic magnets which are β'-$\text{Et}_n\text{Me}_{4-n}\text{X}$ [$\text{Pd}(\text{dmit})_2$]₂ and κ-(BETDT-TTF) systems.</p> <p>ii) Antiferromagnetic La_2CuO_4 and $\text{YBa}_2\text{Cu}_3\text{O}_6$</p> <p>iii) Vanadium thiobromide $\text{V}_4\text{S}_9\text{Br}_4$.</p>	<p>iv) $\text{CeRu}_2\text{Al}_{10}$ which is a Kondo semiconductor and a strongly correlated material.</p> <p>v) Metal-organic hybrid materials which are $(\text{C}_2\text{H}_5\text{NH}_3)_2\text{CuCl}_4$ and $(\text{C}_6\text{H}_5(\text{CH}_2)_2\text{NH}_3)_2\text{CuCl}_4$.</p> <p>vi) Pyrochlore systems such as $\text{Nd}_2\text{Ir}_2\text{O}_7$ and $\text{Sm}_2\text{Ir}_2\text{O}_7$.</p> <p>vii) Organic superconductors such as λ-(BETS)₂GaCl₄.</p> <p>2. Specific usage.</p> <p>Two main software packages were used to conduct our computational studies. They are</p> <p>i) Gaussian 09 for electronic structure and hyperfine interaction calculations.</p> <p>ii) VASP software for band structure and supercell calculations. This software is owned by Advanced Meson Science Laboratory.</p> <p>RICC, MPC, ACSG and ACSL resources at ACCC were used for our computing needs.</p> <p>3. Results</p> <p>We have continued our computational work on the stopping sites and related hyperfine interactions in the systems that we are studying. We have performed further calculations to investigate the density of states and minimum potential sites in $\text{V}_4\text{S}_9\text{Br}_4$ and La_2CuO_4</p>
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In the $\text{YBa}_2\text{Cu}_3\text{O}_6$ system, we have continued our calculations to study the muon stopping sites under conditions where there is lattice relaxation.

For the $\text{Ce}(\text{Ru},\text{Rh})_2\text{Al}_{10}$ system, we have succeeded in calculating the potential energy, dynamic relaxation with and without spin, in a supercell of $\text{CeRu}_2\text{Al}_{10}$ up to $2 \times 2 \times 2$.

We have expanded our calculations on $(\text{C}_2\text{H}_5\text{NH}_3)_2\text{CuCl}_4$ and $(\text{C}_6\text{H}_5(\text{CH}_2)_2\text{NH}_3)_2\text{CuCl}_4$ to bigger supercells in order to study magnetic interactions in far-separated magnetic ions.

We have also performed calculations to study the electronic structure of $\kappa\text{-(BEDT-TTF)}_2\text{Cu}[\text{N}(\text{CN})_2]\text{Cl}$.

We have started performing calculations on the density of states, band structure and minimum potentials on pyrochlore systems, $\text{Nd}_2\text{Ir}_2\text{O}_7$ and $\text{Sm}_2\text{Ir}_2\text{O}_7$ using VASP. And we have been able to estimate the local field at muon sites in these materials using the static-point dipole calculations.

Preliminary studies have also been carried out to study the band structure of the organic superconductor $\lambda\text{-(BETS)}_2\text{GaCl}_4$.

We have been able to further our studies on the $\beta\text{'-Me}_4\text{P}[\text{Pd}(\text{dmit})_2]_2$ system by performing calculations to study the antiferromagnetic ordering in the two-dimensional quasi triangular structure within the dimers.

4. Conclusions

We have been able to carry out the computations that form the basis of our endeavor for studying the electronic and magnetic characteristics of these novel materials. And the results of some of our studies have complemented the experimental results obtained from μSR experiments and have

enabled scientists to better understand these materials. The supercomputing facilities at ACCC have enabled us to conduct such studies.

5. Schedule and prospect for the future

We will need and would like to continue using the ACCC High Performance Computing facilities in our studies on muon in materials. We have received requests from new members to join our group, with new materials to study. For the new FY, we expect to perform further and more complex calculations on the materials that we are currently studying, and also to begin calculations involving new materials.

Fiscal Year 2015 List of Publications Resulting from the Use of the supercomputer**[Publication]**

1. A.F. Rozlan, S. Sulaiman, M.I. Mohamed-Ibrahim, and I. Watanabe; *Electronic Structure of Muonated La_2CuO_4* , Mater. Sci. Forum **827**, 240-242 (2015).
2. I. Watanabe, E. Suprayoga, N. Adam, Mohm-Tajudin S.S., Rozlan A.F., D. Puspita, R. Asih, F. Astuti, M.D. Umar, J. Angel, S. Sulaiman, and M.I. Mohamed-Ibrahim; *Muon Site Estimations by DFT Calculations in Metal and Insulating Systems*, Mater. Sci. Forum **827**, 347-354 (2015).
3. S. Sulaiman, S.N.A. Ahmad, M.I. Mohamed-Ibrahim, and I. Watanabe; *Electronic Structure of Muoniated $Me_4P[Pd(dmit)_2]_2$* , Mater. Sci. Forum **827**, 355-359 (2015).
4. Suprayoga, E., Nugroho, A. A., Polyakov, A. O., Palstra, T. T. M., and Watanabe, I., (2015): Determination of Muon Sites on Metal-Organic Hybrids of $(C_6H_5CH_2CH_2NH_3)_2 CuCl_4$ and $(C_2H_5NH_3)_2CuCl_4$, *RIKEN Accel. Prog. Rep.*, **48**, 267.
5. Mohd-Tajudin, S. S., Ahmad, S. N. A., Hasan-Baseri, D. F. Suprayoga, E., Adam, N., Rozlan, A. F., Sulaiman, S., Mohamed-Ibrahim, M. I., and Watanabe, I., (2015) : An Investigation of Muon Sites in $YBa_2Cu_3O_6$ by Using Density Functional Theory, *RIKEN Accel. Prog. Rep.*, **48**, 268.
6. Adam, N., Suprayoga, E., Adiperdana, B., Guo, H., Tanida, H., Mohd-Tajudin, S. S., Kobayashi, R., Sera, M., Nishioka, T., Matsumura, M., Sulaiman, S., Mohamed-Ibrahim, M. I., and Watanabe, I.; Muon Sites in $Ce(Ru,Rh)_2Al_{10}$ Investigated by Using Density Functional Theory from the View Point of Electronic Potential, *RIKEN Accel. Prog. Rep.*, **48**, 269.

[Others (Press release, Science lecture for the public)]

1. R. Asih, N. Adam, S.S. Mohd. Tajudin, E. Suprayoga, D.P.Sari, K.Matsuhira, M.Wakeshima, Y. Hinatsu, A. Miyake, M. Tokunaga, I. Watanabe, T. Nakano, and Y. Nozue; *μSR study on the pyrochlore iridates on $R_2Ir_2O_7$ ($R = Nd$ and Sm)*, RIKEN-RAL Muon Facility 25-years Operation Celebration and Users Meeting on Feb. 16th-17th, 2016 (poster).
2. D. P. Sari, R. Asih, K. Hiraki, Y. Ishii, H. Kumagai, A. Kawamoto, T. Takahashi, I. Watanabe, T. Nakano, Y. Nozue; *μSR Study of Non-magnetic Anion Based Organic Superconductor*, RIKEN Summer School, Kawagoe-shi, September 4-5, 2015 (poster).
3. D. P. Sari, R. Asih, K. Hiraki, Y. Ishii, H. Kumagai, A. Kawamoto, T. Takahashi, I. Watanabe, T. Nakano, Y. Nozue; *Superconducting Properties of Non-magnetic Anion Based Organic Superconductor λ -(BETS) $_2$ GaCl $_4$ Studied by μSR* , JPS Autumn Meeting 2015, Kansai University, September 16-19, 2015 (oral).
4. D. P. Sari, R. Asih, K. Hiraki, Y. Ishii, H. Kumagai, A. Kawamoto, T. Takahashi, I. Watanabe, T. Nakano, Y. Nozue; *μSR Study of Non-magnetic Anion Based Superconductors λ -(BETS) $_2$ GaCl $_4$* , International Symposium on Present and Future of Material Sciences 2015, Osaka University, November 17-18, 2015 (poster).
5. D. P. Sari, R. Asih, K. Hiraki, Y. Ishii, H. Kumagai, A. Kawamoto, T. Takahashi, I. Watanabe, T. Nakano, Y. Nozue; *μSR Study of Organic Superconductor λ -(BETS) $_2$ GaCl $_4$* , CEMS-APW Workshop, Okachi-Hall RIKEN, January 25-27, 2016 (poster).
6. A.F Rozlan, S.Sulaiman, M.I.M-Ibrahim, I.Watanabe; *Electronic Structure of Muonated La_2CuO_4* , The International RIKEN Symposium: The Frontier of Applications of Muon Science held in the Wako Campus of RIKEN in Japan on 16th and 17th of Feb. in 2016 (poster).

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7. Siti Nur Afifi Ahmad, Harison Rozak, Shukri Sulaiman, Mohamed Ismail Mohamed-Ibrahim, Isao Watanabe; *First Principle Studies on the Electronic Structure of $Me_4P[Pd(dmit)_2]_2$* , RIKEN-RAL Muon Facility 25-years Operation Celebration and Users Meeting on Feb. 16th-17th, 2016 (poster).
8. Dang Fatihah Hasan Baseri, Shukri Sulaiman, Mohamed Ismail Mohamed Ibrahim; *First Principle Computational Studies On The Electronic Structure Of Muoniated κ -(BEDT-TTF) $_2$ Cu[N(CN) $_2$]Cl*, The International RIKEN Symposium: The Frontier of Applications of Muon Science on 16th and 17th of Feb. in 2016 (poster).
9. Saidah Sakinah Mohd-Tajudin, Noraina Adam, Edi Suprayoga, Shukri Sulaiman, Mohamed Ismail Mohamed-Ibrahim and Isao Watanabe; *First principle calculation of electronic structure and muon sites in $YBa_2Cu_3O_6$* , Japan Physical Society 70th Annual Meeting 2015 at Waseda University, 21-Mar-2015 (oral)
10. S.S. Mohd-Tajudin, T. Nishizaki, A Kikkawa, N Adam, E. Suprayoga, S. Sulaiman, M.I. Mohamed-Ibrahim and I. Watanabe; *μ SR and density functional studies on $YBa_2Cu_3O_6$* , Japan Physical Society 2015 Autumn Meeting at Kansai University, 16-Sep-2015 (oral).
11. S.S. Mohd-Tajudin, T. Nishizaki, A Kikkawa, N Adam, E. Suprayoga, S. Sulaiman, M.I. Mohamed-Ibrahim and I. Watanabe; *Study of muon site calculations and experimental in $YBa_2Cu_3O_6$* , Asia-Pacific Workshop (APW)-CEMS Joint Workshop at RIKEN,Wako-shi, 26-Jan-2015 (poster).