

# Sai Mu

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## Education

- ◇ Ph. D, Physics, University of Nebraska-Lincoln, 2008-2014. Advisor: **Kirill D. Belashchenko**  
*Concentration: Condensed matter theory and materials science*
- ◇ B. S., Physics, Beihang University, 2004-2008.

## Employment

- ◇ Assistant Professor, University of South Carolina, 2022/08–present.
- ◇ Associate Specialist, University of California, Santa Barbara, 2020/12–2022/07.  
(Advisor: **Prof. Chris G. Van de Walle**)
- ◇ Postdoctoral Research Associate, University of California, Santa Barbara, 2019/01–2020/11.  
(Advisor: **Prof. Chris G. Van de Walle**)
- ◇ Postdoctoral Research Associate, Oak Ridge National Laboratory, 2015/10–2018/12.  
(Advisor: **Prof. G. Malcom Stocks**)
- ◇ Postdoctoral Research Associate, University of Nebraska-Lincoln, 2015/1–2015/9.  
(Advisor: **Prof. Kirill D. Belashchenko**)
- ◇ Graduate Research Assistant, University of Nebraska-Lincoln, 2010/8–2014/12.  
(Advisor: **Prof. Kirill D. Belashchenko**)

## Research Interests

First-principles methods for the electronic, magnetic and vibrational properties of quantum materials for practical device applications:

- ◇ Multifunctional correlated transition metal oxides with mutually-coupled order parameters, such as magnetoelectric effect, pizeomagnetic effect, etc
- ◇ Magnetic properties (magnetic transition temperature, magnetic anisotropy) of correlated transition metal compounds and heterostructures for spintronics applications
- ◇ Electron, spin and thermal transport in disordered magnetic alloys and high entropy alloys at finite temperatures
- ◇ Phonon scattering and lattice thermal transport in semiconductors
- ◇ Electron and hole transport in semiconductors due to electron-phonon interaction
- ◇ (Quantum) defects in wide bandgap semiconductors for device applications in power electronics and quantum information.

## Skills

- ◇ Stimulating fundamental properties of film, bulk, superlattice, surface/interface etc, via first-principles simulation package: VASP, QUANTUM ESPRESSO, FLEUR, ELK, LMTO, SPR-KKR, LSMS, Wannier90, EPW, LAMMPS, OOMMF
- ◇ Comprehensive knowledge of Linux, numerical programming using Fortran and Python, and scientific softwares including Mathematica and Matlab

## Patent

"Magnetolectric chromia having increased critical temperature", Christian Binek, K. D. Belashchenko, Peter Dowben, **Sai Mu**, A. L. Wysocki, Mike Street, US patent 9718700, 2017/08.

## Awards

- ◇ Outstanding Postdoctoral Researcher Award, Solid State Lighting and Energy Electronics Center (SSLEEC), UCSB (2021)
- ◇ Outstanding Reviewer Award, *Acta Materialia* (2020)
- ◇ Fellowship, Summer School: Electronic Structure Theory for Materials and (Bio)molecules, UCLA, (2014)
- ◇ Travel award, Gordon Conference on Multiferroic and Magnetolectric Materials, University of New England, (2014)

## Publications

### *Under review*

3. Haoxiang Li, A. Said, J. Q. Yan, D. M. Mandrus, H. N. Lee, **Sai Mu**, Yongqiang Cheng, Tom Berlijn, S. Okamoto, Gabor B. Halasz, and H. Miao, "Divergence of Majorana-Phonon Scattering in Kitaev Quantum Spin Liquid"
2. Xun Li, S. Do, J. Yan, M. McGuire, G. Granroth, **Sai Mu**, T. Berlijn, V. Cooper, A. Christianson, L. Lindsay, "Phonons and phase symmetries in bulk  $\text{CrCl}_3$  from scattering measurements and theory"
1. **Sai Mu**, Chris G. Van de Walle, "Phase stability of  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  polymorphs: a first-principles study"

### *Journals*

2022

49. Mengen Wang, **Sai Mu**, Chris Van de Walle, "First-principles studies of diffusion in gallium oxide", Proc. of SPIE, 12002, 120020B-1 (2022). [DOI].
48. Joseph Casamento, Hyunjea Lee, Takuya Maeda, Ved Gund, Kazuki Nomoto, Len van Deurzen, Wesley Turne, Patrick Fay, **Sai Mu**, Chris Van de Walle, Amit Lal, Huili Xing, Debdeep Jena, "Epitaxial  $\text{Sc}_x\text{Al}_{1-x}\text{N}$  on GaN exhibits attractive High-k dielectric properties" *Appl. Phys. Lett.* **120**, 152901 (2022)[DOI].

47. **Sai Mu**, M. Wang, J. Varley, J. Lyon, D. Wickramaratne, Chris G. Van de Walle, "Role of carbon and hydrogen in limiting  $n$ -type doping of monoclinic  $(Al_xGa_{1-x})_2O_3$ " *Phys. Rev. B* **105**, 155201 (2022)[DOI].
46. **Sai Mu**\*, K. D. Dixit\*, Xiaoping Wang, Douglas Abernathy, Stephen E. Nagler, Paula Lampen-Kelley, David Mandrus, C. G. Polanco, L. Liang, Y. Cheng, Arnab Banerjee and Tom Berlijn, "Searching Majorana Fermions in  $\alpha$ - $RuCl_3$  via phonons: the role of the third dimension" (\* Equal Contribution) *Phys. Rev. Res.* **4**, 013067 (2022) [DOI].

#### 2021

45. Xiuli Yang, **Sai Mu**, Hongliang Shi, and Mao-Hua Du, "Theoretical studies of broadband absorption and emission spectra in zero-dimensional mixed-halide perovskite" *J. Appl. Phys.* **130**, 203106 (2021) [DOI]
44. **Sai Mu**, Andrew J. E. Rowberg, Joshua Leveille, Feliciano Giustino, and Chris G. Van de Walle, "First-principles study of electron transport in ScN", *Phys. Rev. B*, **104**, 075118 (2021) [DOI].
43. Mengen Wang, **Sai Mu**, Chris G. Van de Walle, "Incorporation of Si and Sn donors in  $\beta$ - $Ga_2O_3$  through surface reconstructions" *J. Appl. Phys.* **130**, 185703 (2021) (Editor's Pick) [DOI]
42. A. J. E. Rowberg, **Sai Mu**, M. Swift and Chris G. Van de Walle, "Structural, electronic, and polarization properties of YN and LaN" *Phys. Rev. Mater.* **5**, 094602 (2021). [DOI]
41. Hyun Seok Oh, Khorgolkhuu Odbadrakh, Yuji Ikeda, **Sai Mu**, Fritz Kormann, Chengjun Sun, Hye Sang Ahn, Kook Noh Yoon, Duancheng Ma, Cemal Cem Tasan, Takeshi Egami, and Eun Soo Park, "Lattice distortion and atomic-level pressure in  $3d$  complex concentrated alloys" *Acta Materialia*, **216**, 117135 (2021) [DOI]
40. H. Wang, N. Adamski, **Sai Mu**, C. G. Van de Walle "Piezoelectric effect and polarization switching in  $Al_{1-x}Sc_xN$ " *J. Appl. Phys.* **130**, 104101 (2021) (Editor's pick) [DOI]
39. Jingjing Shi, Anusha Krishnan, A F M Anhar Uddin Bhuiyan, Yee Rui Koh, Kenny Huynh, Akhil Mauze, **Sai Mu**, Brian Foley, Ahmad Habib, Takeki Itoh, Yuwei Zhang, Zixuan Feng, Chao Yuan, Samuel Kim, W. Alan Doolittle, Chris Van de Walle, James S. Speck, Mark Goorsky, Patrick Hopkins, Hongping Zhao, Samuel Graham, "Thermal transport across Al- $(Al_xGa_{1-x})_2O_3$  and Al- $Ga_2O_3$  interfaces" *International Electronic Packaging Technical Conference and Exhibition*, **85505**, V001To8A005, 2021.
38. Jared M. Johnson, Hsien-Lien Huang, Mengen Wang, **Sai Mu**, Joel B. Varley, A F M Anhar Uddin Bhuiyan, Zixuan Feng, Nidhin Kurian Kalarickal, Siddharth Rajan, Hongping Zhao, Chris G. Van de Walle, and Jinwoo Hwang "Atomic scale investigation of aluminum incorporation, defects, and phase stability in  $\beta$ - $(Al_xGa_{1-x})_2O_3$  films" *APL Materials* **9(5)** 051103 (2021). [DOI]
37. C. F. Li, K. N. Zhao, X.B. Liao, Z.Y. Hu, L. Zhang, Y. Zhao, **S. Mu**, Y. Li. Y. Li, G. Van Tendeloo, C. Sun "Interface cation migration kinetics induced oxygen release heterogeneity in layered lithium cathodes" *Energy Storage Materials* **36**, 115 (2021)[DOI]
36. Mengen Wang, **Sai Mu**, Chris G. Van de Walle, "Adsorption and diffusion of aluminum on  $\beta$ - $Ga_2O_3$  (010) surfaces" *ACS Appl. Mater. Interfaces* (2021)[DOI]

## 2020

35. **Sai Mu**, Yuewei zhang, Hartwin Peelaers, Mengen Wang, Chris G. Van de Walle, "Orientation-dependent band offsets between and  $(Al_xGa_{1-x})_2O_3$  and  $Ga_2O_3$ " *Appl. Phys. Lett.* **117**, 252104 (2020) (**Editor's pick**). [DOI]
34. **Sai Mu\***, R. J. Olsen\*, B. Dutta\*, L. Lindsay, G. D. Samolyuk, T. Berlijn, E. D. Specht, K. Jin, H. Bei, T. Hickel, B. C. Larson and G. M. Stocks, "Unfolding the complexity of phonon quasi-particle physics in disordered materials" (\* Equal Contribution), *npj Comput. Mater.*, **6**, 4 (2020). [DOI]
33. **Sai Mu**, M. Wang, H. Peelaers, Chris G. Van de Walle, "First-principles surface energies for monoclinic  $Ga_2O_3$  and  $Al_2O_3$  and consequences for cracking of  $(Al_xGa_{1-x})_2O_3$  " *APL Materials*, **8**, 091105 (2020) (**Featured article**). [DOI]
32. A. D. Christianson, V. R. Fanelli, L. Lindsay, **S. Mu**, M. C. Rahn, D. G. Mazzone, A. H. Said, F. Ronning, E. D. Bauer, J. M. Lawrence "Phonons, Q-dependent Kondo spin fluctuations, and  $4f$ /phonon resonance in  $YbAl_3$ " *Phys. Rev. B*, **102**, 205135 (2020). [DOI]
31. Michael W. Swift, Hartwin Peelaers, **Sai Mu**, John J. L. Morton, and Chris G. Van de Walle, "Shallow Donors in Silicon from First Principles: Hyperfine Interaction, Binding Energy, and Quadrupole Coupling", *npj Comput. Mater.* **6**, 181 (2020). [DOI]
30. D. Billington, A.D.N. James, E.I. Harris-Lee, D. O'Neill, N. Tsuda, K. Toyoki, Y. Kotani, T. Nakamura, H. Bei, **Sai Mu**, G.D. Samolyuk, G.M. Stocks, J.A. Duffy, J.W. Taylor, S.R. Giblin, and S.B. Dugdale "Bulk and element specific magnetism of the medium and high entropy Cantor-Wu alloys" *Phys. Rev. B* **102**, 174405 (2020). [DOI]
29. Mengen Wang, **S. Mu**, Chris G. Van de Walle, "Role of Ga and In Adatoms in the epitaxial growth of the  $\beta$ - $Ga_2O_3$ ", *Phys. Rev. B* **102**, 035303 (2020). [DOI]
28. Congli Sun, Xiaobin Liao, Fan-Jie Xia, Yan Zhao, Lei Zhang, **Sai Mu**, Shanshan Shi, Yanxi Li, Haoyang Peng, Tendeloo Gustaaf, Kangning Zhao, Jinsong Wu, "High Voltage Cycling Induced Thermal Vulnerability in Layered Lithium Transition Metal Oxides: Cation Loss and Oxygen Release Driven by Oxygen Vacancy Injection, *ACS Nano*, **14**, 6181 (2020)" [DOI]
27. Z. Pei, **S. Mu**, W. Ming "The local strain distribution in bilayer materials: A multiscale study" , *Nanoscale*, **12**, 6456 (2020) [DOI]
26. Lisha Fan, Xiang Gao, Thomas O. Farmer, Dongkyu Lee, Er-Jia Guo, **S. Mu**, Kai Wang, Michael R. Fitzsimmons, Matthew F. Chisholm, Thomas Z. Ward, Gyula Eres and Ho Nyung Lee, "Vertically Aligned Single-Crystalline  $CoFe_2O_4$  Nanobrush Architectures with High Magnetization and Tailored Magnetic Anisotropy" , *Nanomaterials*, **10**, 472 (2020) [DOI]
25. H. C. Robarts, T. E. Millichamp, D. A. Lagos, J. Laverock, D. Billington, J. A. Duffy, D. O'Neill, S. R. Giblin, J. W. Taylor, G. Kontrym-Sznajd, M. Samsel-Czekala, H. Bei, **S. Mu**, G. D. Samolyuk, G. M. Stocks, and S. B. Dugdale, "Extreme Fermi surface smearing in a maximally disordered alloys" , *Phys. Rev. Lett.*, **124**, 046402 (2020) [DOI]

## 2019

24. **Sai Mu**, K. D. Belashchenko, "Influence of strain and chemical substitution on the magnetic anisotropy of antiferromagnetic  $Cr_2O_3$ : an *ab-initio* study", *Phys. Rev. Mater.* **3**, 034405 (2019). [DOI]

23. **Sai Mu**, G. D. Samolyuk, S. Wimmer, M. C. Tropicovsky, S. Khan, S. Mankovsky, H. Ebert and G. M. Stocks, "Uncovering electron scattering mechanisms in alloys possessing extreme disorder", *npj Computational Materials* **5**,1, (2019). [DOI]
22. **Sai Mu**, H. Peelaers, C. G. Van de Walle, "Ab-initio study of enhanced thermal conductivity in ordered AlGaO<sub>3</sub> alloy", *Appl. Phys. Lett.*, **115**, 242103 (2019). [DOI]
21. G. D. Samolyuk, C. C. Homes, A. F. May, **S. Mu**, K. Jin, H. Bei, G. M. Stocks, B. C. Sales, "Prediction of the Optical Conductivity of metal alloys with residual resistivities near or above the Mott-Ioffe-Regel Limit", *Phys. Rev. B*, **100**, 075128 (2019). [DOI]
20. **Sai Mu**, S. Wimmer, S. Mankovsky, H. Ebert, G. M. Stocks "Influence of local lattice distortions on electrical transport of refractory high entropy alloys", *Scr. Mater.* **170**, 189 (2019). [DOI]
19. H. S. Oh, S. J. Kim, K. Odbadrakh, W. H. Ryu, K. N. Yoon, **S. Mu**, F. Körmann, Y. Ikeda, C. C. Tasan, D. Raabe, T. Egami, E. S. Park, "Engineering atomic-level complexity in high-entropy and complex concentrated alloys", *Nat. Commun.* **10**, 2090 (2019). [DOI]
18. M. A. McGuire, T. Pandey, **S. Mu**, and D. S. Parker, "Ferromagnetic spin-1/2 dimers with strong anisotropy in MoCl<sub>5</sub>", *Chem. Mater.* **31**, 2952, (2019). [DOI]
17. **Sai Mu**, R. P. Hermann, S. Gorsse, H. Zhao, M. E. Manley, R. S. Fishman, L. Lindsay, "Phonons, magnons and lattice thermal transport in antiferromagnetic semiconductor MnTe" *Phys. Rev. Mater.* **3** (2), 025403, (2019). [DOI]
16. **Sai Mu**, J. Yin, G. D. Samolyuk, S. Wimmer, Z. Pei, M. Eisenbach, S. Mankovsky, H. Ebert and G. M. Stocks, "Hidden Mn magnetic-moment disorder and its influence on the physical properties of medium-entropy NiCoMn alloy ", *Phys. Rev. Mater.* **3**, 014411, (2019). [DOI]

## 2018

15. **Sai Mu**, Zongrui Pei, Xianglin Liu, G. M. Stocks, "Electronic transport and phonon properties of maximally disordered alloys: from binaries to high entropy alloys", *J. Mater. Res.* **33**, 2857 (2018). [DOI] [invited review]
14. D. Meyers, K. Nakatsukasa, **Sai Mu**, L. Hao, J. Yang, Y. Cao, G. Fabbris, H. Miao, J. Pellicciari, D. McNally, M. Dantz, E. Paris, E. Karapetrova, Yongseong Choi, D. Haskel, Jian Liu, Thorston Schmitt, S. Johnston, Tom Berlijn, and M. P. M. Dean, "Decoupling carrier concentration and electron-phonon coupling in oxide heterostructures" *Phys. Rev. Lett.* **121**, 236802, (2018). [DOI]
13. Z. Pei, M. Eisenbach, **S. Mu**, and G. M. Stocks, "Error controlling of the combined Cluster-Expansion and Wang-Landau Monte-Carlo method and its application to FeCo", *Comput. Phys. Commun.* **235**, 95, (2018). [DOI]
12. G. D. Samolyuk, **Sai Mu**, A. F. May, B. C. Sales, S. Wimmer, S. Mankovsky, H. Ebert, G. M. Stocks, "Temperature dependent electronic transport in concentrated solid solutions of the 3d-transition metals Ni, Fe, Co and Cr from first principles", *Phys. Rev. B* **98**,165141, (2018). [DOI]
11. Xin Zhang, **S. Mu**, Yang Liu, Jian Luo, Jian Zhang, Alpha T. N'Diaye, Axel Enders, and Peter A. Dowben, "The Electronic Structure Signature of the Spin Cross-Over Transition of [Co(dpzca)<sub>2</sub>]", *Z. Phys. Chem.* **232**(4) 445 (2018). [DOI]
10. D. Li, Z. Xiao, **S. Mu**, F. Wang, Y. Liu, J. Song, X. Huang, L. Jiang, J. Xiao, L. Liu, S. Ducharme, B. Cui, X. Hong, L. Jiang, J. Silvain, and Y. Lu, "A Facile Space-Confined Solid-Phase Sulfurization Strategy for Growth of High-Quality Ultrathin Molybdenum Disulfide Single Crystals", *Nano Lett.* **18**(3), 2021 (2018). [DOI]

**2017**

9. L K Béland, A Tamm, **S. Mu**, G. D Samolyuk, Y. N Osetstky, A Aabloo, A Caro, M Klintonberg, R. E Stoller, "Accurate classical short-range forces for the study of collision cascades in Fe-Ni-Cr", *Comput. Phys. Commun.* **219**, 11 (2017). [DOI]
8. F. X. Zhang, K. Jin, S. Zhao, **S. Mu**, H. Bei, J. C. Liu, H. Z. Xue, D. Popov, C. Park, G. M. Stocks, W. J. Weber, Y. Zhang, "X-ray absorption investigation of local structural disorder in Ni<sub>1-x</sub>Fe<sub>x</sub> (x = 0.10, 0.20, 0.35 and 0.5) alloys", *J. Appl. Phys.* **121**, 165105, (2017). [DOI]

**2016**

7. K. Jin, **Sai Mu**, K. An, W. Porter, G. Samolyuk, G. M. Stocks and H. Bei, "Thermophysical properties of Ni-containing single-phase concentrated solid solution alloys", *Mater. Des.* **117**, 185 (2016). [DOI]
6. Sumit Beniwal, Xin Zhang, **S. Mu**, Patrick Rosa, Guillaume Chastanet, Jean-Francois Letard, Jing Liu, George E. Sterbinsky, Dario A. Arena, Peter A. Dowben, Axel Enders, "Substrate-induced spin state locking of the [Fe(H<sub>2</sub>B(pz)<sub>2</sub>)<sub>2</sub>(bipy)] spin crossover complex", *J. Phys.: Condens. Matter.* **28**, 206002 (2016). [DOI]

**2015**

5. K. D. Belashchenko, J. Weerasinghe, **Sai Mu**, B. Pujari, "Spectral signatures of thermal spin disorder and excess Mn in half-metallic NiMnSb", *Phys. Rev. B* **91**, 180408(R) (2015) [*rapid communication*]. [DOI]
4. Xin Zhang, **Sai Mu**, Tatiana Palamarciuc, Patrick Rosa, Jean-Francois Letard, Jing Liu, Dario Arena, Bernard Doudin, Peter A. Dowben, "Complexities in the molecular spin crossover transition", *J. Phys. Chem. C* **119** (28), 16293 (2015). [DOI]
3. **Sai Mu**, K. D. Belashchenko, "Strategies for increasing the Néel temperature of magnetoelectric Fe<sub>2</sub>TeO<sub>6</sub>", *J. Phys.: Condens. Matter.* **27**, 022203 (2015) [*fast track communication*]. [DOI]

**2014**

2. **Sai Mu**, A. L. Wysocki, K. D. Belashchenko, "First-principles microscopic model of exchange-driven magnetoelectric response with application to Cr<sub>2</sub>O<sub>3</sub>", *Phys. Rev. B* **89**, 174413 (2014). [DOI]

**2013**

1. **Sai Mu**, A. L. Wysocki, K. D. Belashchenko, "Effect of substitutional doping on the Néel temperature of Cr<sub>2</sub>O<sub>3</sub>", *Phys. Rev. B* **87**, 054435 (2013). [DOI]

## Presentations

1. (Invited Talk) **Sai Mu**, "Exploring Electron Scattering and Lattice Vibrations in Disordered Concentrated Solid Solution and High Entropy Alloys", CNMS User Meeting, Oak Ridge National Laboratory, Aug, 2022.

2. (Talk) **Sai Mu** *et al.*, "Role of carbon and hydrogen in limiting  $n$ -type doping of monoclinic  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$ ", APS March meeting, 2022.
3. (Invited Talk) **Sai Mu**, "Harnessing Disorder to Tune, Tailor and Design Novel Transition Metal Compounds", Seminar of University of South Carolina, Feb, 2022.
4. (Invited Talk) **Sai Mu** "First-principles surface calculations for monoclinic  $\text{Ga}_2\text{O}_3$  and  $\text{Al}_2\text{O}_3$  and consequences for cracking of  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  films", SPIE conference, 2021.
5. (Talk) **Sai Mu** "First-principles surface calculations for monoclinic  $\text{Ga}_2\text{O}_3$  and  $\text{Al}_2\text{O}_3$  and consequences for cracking of  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  films", APS March meeting, 2021.
6. (Invited Talk) **Sai Mu**, "Exploring Electron Scattering and Lattice Vibrations in Disordered Concentrated Solid Solution and High Entropy Alloys", Seminar of Iowa state university and AMES Lab, Oct, 2019.
7. (Talk) **Sai Mu**, L. Lindsay, R. Olsen, B. C. Larson, G. M. Stocks, "First-principles study of lattice thermal conductivity in concentrated solid solution alloys", APS march meeting, Boston, 2019.
8. (Invited Talk) **Sai Mu** *et al.*, "Effect of Extreme Disorder on the Phonon Scattering in magnetic binary alloys", TMS meeting, Phoenix, 2018.
9. (Talk) **Sai Mu**, *et al.*, "Effect of Extreme Disorder on the Lattice Dynamics and Phonon Scattering in Concentrated Solid Solution Alloys", APS march meeting, Los Angeles, 2018.
10. (Poster) **Sai Mu**, G. D. Samolyuk, S. Wimmer, Sergiy Mankovsky, S. Khan, C. Troparevsky, E. Hubert, and G. M. Stocks, "Electronic transport in concentrated magnetic alloys" ES 2017 workshop, Princeton University, 2017.
11. (Talk) **Sai Mu**, G. D. Samolyuk, S. Wimmer, Sergiy Mankovsky, S. Khan, C. Troparevsky, E. Hubert, and G. M. Stocks, "Uncovering Electron Scattering Mechanisms in Concentrated Solid Solution Alloys", APS march meeting, New Orleans, 2017.
12. (Talk) **Sai Mu**, G. D. Samolyuk, S. Wimmer, Sergiy Mankovsky, S. Khan, C. Troparevsky, S. Zhao, M. Daene, and G. M. Stocks, "First-principles study of the residual resistivity of single-phase Ni-based high entropy alloys", MMM, New Orleans, 2016.
13. (Talk) **Sai Mu**, Kirill Belashchenko, "Aspects of bulk and surface magnetism of magnetoelectric  $\text{Fe}_2\text{TeO}_6$ ", APS march meeting, San Antonio, 2015.
14. (Talk) **Sai Mu**, Kirill Belashchenko, "First-principles study of the magnetic properties of  $\text{Fe}_2\text{TeO}_6$  towards increasing its Néel temperature", MMM, Honolulu, 2014.
15. (Poster) **Sai Mu**, Aleksander Wysocki, Kirill Belashchenko, "Towards higher Néel temperature and exchange-driven magnetoelectric response in  $\text{Cr}_2\text{O}_3$ : An *ab initio* study", Gordon Research Conference: Multiferroics and magnetoelectric materials, 2014.
16. (Poster) **Sai Mu**, Kirill Belashchenko, "First-principles studies of the piezomagnetic effect in transition-metal fluorides", APS march meeting, Denver, 2014.
17. (Talk) **Sai Mu**, Aleksander Wysocki, Kirill Belashchenko, "Longitudinal magnetoelectric susceptibility of  $\text{Cr}_2\text{O}_3$ : First-principles calculations using the converse approach", APS march meeting, Baltimore, 2013.
18. (Talk) **Sai Mu**, Kirill Belashchenko, "First-principles studies of the piezomagnetic effect in transition-metal fluorides  $\text{MF}_2$  ( $M = \text{Mn}, \text{Fe}, \text{Co}$ )", MMM, Dever, 2013.

19. (Poster) **Sai Mu**, Aleksander Wysocki, Kirill Belashchenko, "Prospects of increasing the Néel temperature of  $\text{Cr}_2\text{O}_3$ : An *ab initio* study", SRC TECHCON, Austin, 2013.
20. (Poster) **Sai Mu**, Aleksander Wysocki, Kirill Belashchenko, "Prospects of increasing the Néel temperature of  $\text{Cr}_2\text{O}_3$ : An *ab initio* study", CNFD onsite review, Lincoln, 2013.
21. (Poster) **Sai Mu**, Aleksander Wysocki, Kirill Belashchenko, "Effect of doping and strain on Néel temperature of  $\text{Cr}_2\text{O}_3$ : An *ab initio* study", APS march meeting, Dallas, 2011.