Vamshi Mohan Katukuri

Date of Birth: 30 March 1983
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Education

- **PhD - Physics (Condensed matter theory)**

  Magna Cum Laude - Technische Universität Dresden , Dresden, Germany
  Apr 2011 - Feb 2015
  Advisor: **Prof. Jeroen van den Brink** (Defended on 5th Feb 2015)

- **Master of Science in Material science engineering**

  University of Minnesota (U of M), Twin cities, Minneapolis, USA **Sept 2007 – Sept 2010**
  GPA -- 3.14/4.00

- **Master of Technology in Computational Physics**

  University of Hyderabad, Hyderabad, India **Sept 2005 – Mar 2007**
  CGPA – 9.17/10.00

- **Bachelor and Master of Science in Physics (Photonics)**

  Sri Sathya Sai Institute of Higher Learning, Puttaparthi, India **Jun 2000 – Mar 2005**
  CGPA – 4.39/5.00 (B.Sc), **4.84/5.00** (M.Sc)

Employment

- **Postdoctoral research scientist in C3MP headed by Prof. Oleg Yazvev** **Feb 2015 – Current**
  Institute of Physics, École polytechnique Fédéral de Lausanne, Lausanne, Switzerland
- **Research assistant in the group of Prof. Matteo Cococcioni** **May 2009 – Mar 2011**
  Chemical Engineering and Material Science department **,** University of Minnesota, Minnesota, USA

Organisational activities

- Member of the organising committee for "NCCR MARVEL junior retreat - 2017" **July 2017**

Approved research projects

- RIKEN Special Post Doctoral Researcher fellowship for the years 2016-2018 : A two-year research grant for investigations of magnetic interactions in transition metal oxides (Not taken up).

Research supervision

- Supervised semester projects for master students at EPFL during the years 2015 and 2016

Teaching experience

- Guest lectures on *ab initio* calculation of electronic structure of materials for the doctoral course "General aspects of the electronic structure of crystals" at EPFL **Fall 2017**
- TP4 semester projects (EPFL) **Fall 2015, Fall and Spring 2016**
- ChEn 4201: Numerical methods in chemical engineering applications (U of M) **Spring 2008**
- MatS 3011: Introduction to material science engineering (U of M) **Fall 2008**

Scientific journal review activity

Reviewer of

- Physical Review Letters
- Physical Review B: Condensed Matter Physics
- Journal of Physics: Condensed Matter
- Communications Physics (Nature)

Personal and Research Skills

- **Languages:**
  Proficient in English, Telugu and Hindi. Working knowledge in German.
- **Electronic structure calculations:**
  Experience with multiple Quantum chemistry wave function based and Density functional based electronic structure codes, like, **PYSCF**, ***MOLPRO, ORCA,*** (wave function) and ***CRYSTAL, QUANTUM ESPRESSO, YAMBO, WIEN2k, FPLO, PARSEC*** and ***VASP.***
- **Model Hamiltonian calculations:**
  Experience in construction of Tight-Binding and effective Hamiltonians from *ab initio* calculations, mapping onto model Hamiltonians and extracting parameters that help to understand the physics in real materials.
- **Parallel programming:**
  Implemented MPI parallelization on Monte-Carlo program. Identified the most time consuming parts of the electronic structure code named ***PARSEC*** and ***CPMD***, and implemented OpenMP directives in respective programs on shared memory systems.
- **Programming tools and languages:**
  MATHEMATICA, MATLAB, C, FORTRAN, Python, BASH, MPI, OpenMP.

Publications

Total: 20; Citations: 734; h-index: 12

1. "Observation of heavy spin-orbit excitons propagating in a nonmagnetic background: The case of (Ba, $Sr)_2YIrO_6$"
   M. Kusch, **V. M. Katukuri,** N. A. Bogdanov, B. Büchner, T. Dey, D. V. Efremov, J. E. Hamann-Borrero, B. H. Kim, M. Krisch, A. Maljuk, M. Moretti Sala, S. Wurmehl, G. Aslan-Cansever, M. Sturza, L. Hozoi, J. Van Den Brink, J. Geck Phys. Rev. B 96, 104308 **(2018)**

2. "Coherent generation of symmetry-forbidden phonons by light-induced electron-phonon interactions in magnetite"
S. Borroni, E. Baldini, **V. M. Katukuri**, A. Mann, K. Parlinski, D. Legut, C. Arrell, F. van Mourik, J. Teyssier, A. Kozlowski, P., O. V. Yazyev, A. M. Oleś, J. Lorenzana, F. Carbone Phys. Rev. B 96, 104308 **(2017)**

3. "J_1 — J_2 square lattice antiferromagnetism in the orbitally quenched insulator $MoOPO_4$"
L. Yang, M. Jeong, P. Babkevich, **V. M. Katukuri**, B. Náfrádi, N. E. Shaik, A. Magrez, H. Berger, J. Schefer, E. Ressouche, M. Kriener, I Živković, O. V. Yazyev, L. Forró, H. M. Rønnow Phys. Rev. B 96, 024445 **(2017)**

4. "Doping Dependence of Collective Spin and Orbital Excitations in the Spin-1 Quantum Antiferromagnet $La_{2-x}Sr_xNiO_4$ Observed by X-Rays"
G. Fabbris, D. Meyers, L. Xu, **V. M. Katukuri**, L. Hozoi, X. Liu, Z-Y. Chen, J. Okamoto, T. Schmitt, A. Uldry, B. Delley, G. D. Gu, D. Prabhakaran, A. T. Boothroyd, J. Van Den Brink, D. J. Huang, M. P. M. Dean Phys. Rev. Lett. 118, 156402 **(2017)**

5. "Possible unusual spin state of Ir^{4+} in $Ba_{21}Ir_9O_{43}$ single crystal"
L. Yang, M. Jeong, A. Arakcheeva, I. Živković, B. Náfrádi, A. Magrez, A. Pisoni, J. Jacimovic, **V. M. Katukuri**, S. Katrych, N. E. Shaik, O. V. Yazyev, L. Forró, H. M. Rønnow Phys. Rev. B 94, 104403 **(2016)**

6. "Magnetic excitations and electronic interactions in Sr_2CuTeO_6: a spin-1/2 square lattice Heisenberg antiferromagnet"
P. Babkevich, **V. M. Katukuri**, B. Fåk, S. Rols, T. Fennell, D. Pajić, H. Tanaka, T. Pardini, R. R. P. Singh, A. Mitrushchenkov, O. V. Yazyev, H. M. Rønnow Phys. Rev. Lett 117, 237203 **(2016)**.

7. "Spin-orbit excitation energies, anisotropic exchange, and magnetic phases of honeycomb $RuCl_3$"
R. Yadav, N. Bogdanov, **V. M. Katukuri,**, S. Nishimoto, J. van den Brink and L. Hozoi *Sci. Rep. 6, 37925* **(2016)**.

8. "The vicinity of hyper-honeycomb β-Li_2IrO_3 to a three-dimensional Kitaev spin liquid state"
V. M. Katukuri, R. Yadav, S. Nishimoto, J. van den Brink and L. Hozoi *Sci. Rep. 6, 29585* **(2016)**.

9. "Strongly frustrated triangular spin lattice emerging from triplet dimer formation in honeycomb Li_2IrO_3"
S. Nishimoto, **V. M. Katukuri,** V. Yushankhai, H. Stoll, Ulrich K. Rößler, L. Hozoi, I. Rousochatzakis and J. van den Brink *Nat. commun. 7, 10273* **(2016)**.

10. "Strong magnetic frustration and anti-site disorder causing spin-glass behaviour in honeycomb Li_2RhO_3"
V. M. Katukuri, S. Nishimoto, L. Hozoi and J. van den Brink, *Sci. Rep. 5, 14718* **(2015)**.

11. "Orbital reconstruction in non-polar tetravalent transition-metal oxide layers"
N. A. Bogdanov **V. M. Katukuri,** V. Kataev, Judit Romhanyi, B. Büchner, J. van den Brink and L. Hozoi *Nat. Commun. 6, 7306* **(2015)**.

12. "Mechanism of basal-plane antiferromagnetism in the spin-orbit driven iridate Ba_2IrO_4"
V. M. Katukuri, V. Yushankhai, L. Siurakshina, I. Rousochatzakis, L. Hozoi and J. van den Brink *Phys. Rev. X 4, 021051* **(2014)**.

13. "Electronic structure of low-dimensional $4d^5$ oxides: interplay of ligand distortions, overall lattice anisotropy, and spin-orbit interactions"
V. M. Katukuri, K. Roszeitis, V. Yushankhai, A. Mitrushchenkov, H. Stoll, M. van Veenendaal, P. Fulde, J. van den Brink and L. Hozoi *Inorg. Chem 53(10) 4833* **(2014)**.

14. "Tuning Magnetic Coupling in Sr_2IrO_4 Thin Films with Epitaxial Strain"
A. Lupascu, J. Clancy, H. Gretarsson, Zixin Nie, J. Nichols, J. Terzic, G. Cao, S. Seo, Z. Islam, M. Upton, J. Kim, A. Said, D. Casa, T. Gog, **V. M. Katukuri**, H. Stoll, L. Hozoi, J. van den Brink and Y.-J. Kim *Phys. Rev. Lett. 112 147201* **(2014)**.

15. "Kitaev interactions between j=1/2 moments in honeycomb Na_2IrO_3 are large and ferromagnetic: insights from ab initio quantum chemistry calculations"
V. M. Katukuri, S. Nishimoto, V. Yushankhai, A. Stoyanova, H. Kandpal, Sungkyun Choi, R Coldea, I. Rousochatzakis, L. Hozoi, and J. van den Brink:, *New J. Phys. 16 013056* **(2014)**.

16. "Crystal-field splitting and correlation effect on the electronic structure of A_2IrO_3"
H. Gretarsson, J. P. Clancy, X. Liu, J. P. Hill, E. Bozin, Y. Singh, S. Manni, P. Gegenwart, J. Kim, A. H. Said, D. Casa, T. Gog, M.H. Upton, H.-S. Kim, J. Yu, **V. M. Katukuri**, L. Hozoi, J. van den Brink, and Y.-J. Kim *Phys. Rev. Lett. 110 076402* **(2013)**.

17. "Post-perovskite $CaIrO_3$: A j=1/2 quasi-one-dimensional antiferromagnet"
N.A. Bogdanov, **V. M. Katukuri**, H. Stoll, J. van den Brink, and L. Hozoi *Phys. Rev. B 85 235247* **(2012)**.

18. "Ab initio determination of excitation energies and magnetic couplings in correlated quasi-two-dimensional iridates"
V. M. Katukuri, H. Stoll, J. van den Brink and L. Hozoi *Phys. Rev. B 85 220402* **(2012)**.

19. "Testing the validity of the strong spin-orbit-coupling limit for octahedrally coordinated iridate compounds in a model system Sr_3CuIrO_6"
X. Liu, **V. M. Katukuri**, L. Hozoi, W.-G. Yin, M. P. M. Dean, M. H. Upton, J. Kim, D. Casa, A. Said, T. Gog, T.F. Qi, G. Cao, A.M. Tsvelik, J. van den Brink, J.P. Hill *Phys. Rev. Lett. 109 157401* **(2012)**.

20. "Origin of magnetic interactions and their influence on the structural properties of Ni_2MnGa and related compounds"
B. Himmetoglu, **V. M. Katukuri**, M. Cococcioni *J. Phys.: Cond. Matt. 24 (18), 185501* **(2012)**.

Oral Presentations

Invited Talks

1. "*Ab initio* analysis of magnetic interactions in transition metal oxides: Cuprates, Molybdates and Iridates" - **Max Planck Institute for solid state research**, Stuttgart — May 2017
2. "Material realisation of the Kitaev model on the honeycomb lattice" - **NCCR MARVEL junior seminar at Swiss Federal Institute of Technology Lausanne** (EPFL), Lausanne — Apr 2017
3. "Novel ground states driven by electronic correlations and spin orbit interactions in $5d^5$ iridates: a quantum chemical perspective" — **Indian Institute of Technology - Hyderabad**, Hyderabad — Jun 2016

4. "*Ab initio* quantum chemical approach to spin-orbit excitations and magnetic interactions in 4*d* and 5*d* transition metal compounds" - **Mott physics beyond Heisenberg model, Swiss Physical Society meeting**, Lugano — Aug 2016
5. "Wave function based methods for the study of electronic and magnetic excitations in transition metal oxides" - **Computational condensed matter physics seminar, RIKEN**, Tokyo, Japan — Aug 2015
6. "Anisotropic magnetic interactions driven by spin-orbit coupling in iridium oxides" - **Institute of Theoretical Physics seminar - EPFL**, Lausanne — Sep 2014

Contributed Conference Talks

7. "Topological electronic states in spin-orbit coupled $j_{\text{eff}} = 0$ ground state compound $Ba_3CaIr_2O_9$" - **American Physical Society spring meeting** – Denver, USA — Mar 2018
8. "Spin-orbit enhanced correlations and novel magnetic ground states and excitations in 5d oxides" - **ETSF Young researchers meeting 2016**, Kings college London, UK — Jun 2016
9. " Anisotropic magnetic interactions in 5d iridium oxides by many-body quantum chemistry calculations" - **American Physical Society spring meeting** – Denver, USA — Mar 2014
10. "Spin-orbit excitation in quasi 2D square lattice iridates" **Deutsche Physikalische Gesellschaft spring meeting** – Regensburg, Germany — Mar 2013
11. "Correlated *ab initio* methods for description of RIXS excitations in solids" **Deutsche Physikalische Gesellschaft spring meeting** – Berlin, Germany — Mar 2012

Poster presentations

1. "Magnetic interactions in transition metal oxides: Cuprates, Molybdates and Iridates — from *ab initio* wave function theory" **Quantum-chemistry methods for materials science — CECAM workshop, Lausanne,** Switzerland — Nov 2017
2. "Interrelation of crystal structure and topological non- trivial electronic states in quasi-one-dimensional bismuth halides" **New trends in Topological insulators 2017 — Congressi Stefano Franscini, Monte Verità**, Switzerland — Jul 2017
3. "Kitaev interactions in honeycomb iridates and ruthenates" **Deutsche Physikalische Gesellschaft spring meeting —2015, Berlin**, Germany — Mar 2015
4. "Anisotropic magnetic interactions in $5d^5$ honeycomb and square-lattice iridates" - **Conference on Strongly Correlated Electron System 2014 – Grenoble**, France — Jul 2014
5. "*Ab initio* quantification of anisotropic magnetic interactions in iridium oxides" - **Electronic properties of spin-orbit driven oxides – IFW Dresden**, Germany — Sep 2013
6. "Spin orbit coupling in iridium oxide compounds" - **Fundamental aspects of X-ray spectroscopies: role of 2*p* core hole in XAS and XPS – Utrecht**, Netherlands — Feb 2013
7. "Excitation energies and magnetic couplings in correlated Ir $5d^5$ oxides" - **48th Symposium on Theoretical Chemistry – Karlsruhe**, Germany — Sep 2012

8. “Excitation energies and magnetic couplings in correlated Ir 5d^5 oxides: a quantum chemical study” - **Itinerant spin-orbital systems: magnetic frustration to novel superconductivity – MPI-PKS Dresden**, Germany — May 2012
9. “Ab initio quantum chemistry methods for solids” **Summer school on CRYSTAL quantum chemistry program - Torino**, Italy — Sep 2011