

Dr. Gul Rahman

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PERSONAL

Citizen: Pakistani
Sex and Martial Status: Male and Married

EDUCATION

Ph.D. Physics, February 2008
Department of Physics, University of Ulsan, Ulsan, Republic of Korea.
Ph.D. Thesis: *Half metallicity of artificial zinc blende materials and possible magnetism of non-magnetic materials: Density Functional Study.*

M.Phil. Physics, 2003
Department of Physics, Quaid-e-Azam University, Islamabad, Pakistan.
M.Phil. Thesis: *Effect of La substitutions in CMR (Colossal Magnetoresistnace) compounds.*

M.Sc. Physics, 2000
Department of Physics, University of Peshawar, Peshawar (NWFP), Pakistan.
M.Sc. Thesis: *Dielectric constant of liquids.*

B.Sc. Physics and Mathematics, 1997
Govt. Postgraduate College Mardan, Mardan (NWFP), Pakistan.

RESEARCH EXPERIENCE

March 2008–June 2010, Postdoctoral fellow, Computational Metallurgy:
Graduate Institute of Ferrous Technology, POSTECH, Pohang, Republic of Korea.

2004–2008, Electronic structure calculations: Computational Physics Lab.
Department of Physics, University of Ulsan, Ulsan, Republic of Korea.

2001–2003, Experimental magnetism: Magnetism and Superconductivity Lab.
Department of Physics, Quaid-e-Azam University, Islamabad, Pakistan.

WORK EXPERIENCE

August 2010, Asistant Prof. Department of Physics, Quaid-i-Azam University
(QAU), Islamabad, Pakistan.

2003, Physics lecturer: Aga Khan Higher Secondary School Gilgit, Pakistan.

MEMBERSHIPS AND AWARD

Associate Member of National Centre for Physics (NCP), Islamabad, Pakistan.
Member of The Korean Physical Society (KPS).
Member of The Korean Magnetic Society (KMS).
Merit scholarship on M.Phil level at Quaid-e-Azam University Islamabad, Pakistan.

REVIEWER

Reviewer for *Physica B*
Reviewer for *Nanoscale*
Reviewer for *Physica status solidi*

Reviewer for *Solid State Sciences*
Reviewer for *Applied Surface Science*

INTERNATIONAL COLLABORATIONS	<p>Víctor M. García-Suárez: Department of Physics, Lancaster University, Lancaster, U.K.</p> <p>A. J. Freeman: Department of Physics and Astronomy, Northwestern University, Evanston, U.S.A.</p> <p>H. K. D. H. Bhadeshia: Department of Materials Science and Metallurgy, University of Cambridge, U.K.</p> <p>I. G. Kim: Graduate Institute of Ferrous Technology, Pohang University of Science and Technology, Republic of Korea.</p> <p>J. M. Morbec: Instituto de Ciencias Exatas, Universidade Federal de Alenas, Alenas, Brazil.</p>
FIELDS OF INTEREST	<p>Diluted magnetic semiconductor.</p> <p>New magnetic materials for spintronics (Digital alloys, Superlattices, etc.).</p> <p>Ferromagnetism of oxides and role of defects.</p> <p>Surface and interface magnetism.</p> <p>Nanomagnetism (Nanotubes and Nanoribbons).</p> <p>Mechanical properties of materials.</p> <p>Fe-based Superconductivity.</p> <p><i>Multiferroics, (hobby).</i></p>
COURSE TAUGHT AT QAU	<p>Magnetism and magnetic materials; graduate level course Books: <i>Magnetism in Condensed Matter</i>, by Stephen Blundell, <i>The Physical Principles of Magnetism</i> by Allan H. Morrish, <i>Introduction to magnetic materials</i>, by B. D. Cullity, C. D. Graham.</p> <p>Condensed Matter Physics I; undergraduate Books: <i>Introduction to Solid State Physics</i>, by Charles Kittel, <i>Solid State Physics</i>, by Ashcroft, Neil W., and N. David Mermin, <i>Elementary Solid State Physics: Principles and Applications</i>, by M. Ali Omar, <i>Solid State Physics</i>, by J. R. Hook and H. E. Hall.</p> <p>Condensed Matter Physics II; undergraduate Books: <i>Introduction to Solid State Physics</i>, by Charles Kittel, <i>Solid State Physics</i>, by Ashcroft, Neil W., and N. David Mermin, <i>Elementary Solid State Physics: Principles and Applications</i>, by M. Ali Omar, <i>Solid State Physics</i>, by J. R. Hook and H. E. Hall.</p> <p>Mathematical Methods and Computational Physics ; undergraduate Books: <i>Mathematical Methods for Physicists</i>, by G. Arfken, <i>Numerical Methods for Engineers</i>, by S. C. Chapra and R. Canale.</p>
STUDENT UNDER SUPERVISION	<p>1. Two MS students under supervision</p>
SKILLS	<p>Programming skill in Fortran 77/90 and various utility script languages in UNIX and LINUX systems. Data visualization packages, Gnuplot, Xmgr, and Xcryden for plotting and basic analysis.</p> <p>Various numerical algorithms to solve numerical problems, i.e., iteration methods for solving integral equations, interpolation and extrapolation methods etc.</p>
COMPUTATIONAL METHODS	<p>All-electron, Full Potential Linearized Augmented Plane Wave (FLAPW).</p> <p>Pseudopotential with plane waves, Vienna ab initio simulation package (VASP).</p> <p>Pseudopotential with atomic orbital basis, Spanish Initiative for Electronic Simulations with Thousands of Atoms (SIESTA).</p>
PUBLICATIONS	

1. A first-principles investigation on the effects of magnetism on the Bain transformation of α -phase FeNi systems
Gul Rahman, In Gee Kim, and H. K. D. H. Bhadeshia *J. Appl. Phys.* (2012) **Accepted**.
2. *Ab initio* prediction of pressure-induced structural phase transition of superconducting FeSe
Gul Rahman, In Gee Kim, and A. J. Freeman *J. Phys.: Condens. Matter* (2012) **Accepted**.
3. *Ab-initio* study on magnetism of Al impurity in bcc Fe
Gul Rahman and In Gee Kim *J. Magnetism* **16**, 1 (2011)
4. First-principles prediction of spin-density-reflection symmetry driven magnetic transition of CsCl-type FeSe
Gul Rahman, In Gee Kim, and A. J. Freeman, *J. Magn. Magn. Mater.* **322** 3153 (2010).
5. A systematic study on iron carbides from first-principles
In Gee Kim, **Gul Rahman**, Jae Hoon Jang, You Young Song, Seung-Woo Seo, H. K. D. H. Bhadeshia, A. J. Freeman, and G. B. Olson *Materials Science Forum* **654-656** 47-50 (2010).
6. Magnetism and electronic structures of 3d transition-metal impurities in bcc Fe: A first-principles study
Gul Rahman, In Gee Kim, H. K. D. H. Bhadeshia, and A. J. Freeman *Phys.Rev.B* **81** 184423 (2010).
7. Strain-induced half metallic ferromagnetism in zinc blende CrP/MnP superlattice: First-principles study
Gul Rahman, *Phys.Rev.B* **81**, 124410 (2010).
8. Surface-induced magnetism in C-doped SnO₂
Gul Rahman and Víctor M. García-Suárez *Appl.Phys.Lett.* **96**, 052508 (2010).
9. A Convergence Test of the Full-potential Linearized Augmented Plane Wave (FLAPW) Method: Ferromagnetic BCC Bulk Fe
Seung-Woo Seo, You Young Song, **Gul Rahman**, In Gee Kim, Michael Weinert, and A. J. Freeman *J. Magnetism* **14**, 137 (2009).
10. Magnetic and electronic structure calculations of Antiferromagnetic Mn₂As
Gul Rahman, *J. Magn. Magn. Mater.* **321**, 2775 (2009).
11. Magnetic Properties of Anti-perovskite Tetracobalt Nitride Surfaces: A First-principles Study
Gul Rahman, In Gee Kim, Lee-Hyun Cho, Beata Bialek and Jae Il Lee, *J. Korean. Phys. Soc.* **54**, 145 (2009).
12. A First-principles Study on Magnetic and Electronic Properties of Ni Impurity in bcc Fe
Gul Rahman and In Gee Kim, *J. Magnetism* **13**, 124 (2008).
13. A First-principles Study on the Effects on Magnetism of Si Impurity in BCC Fe by Considering Spin-orbit Coupling
Gul Rahman, In Gee Kim, and Sam Kyu Chang, *J. Korean Magnetic Soc.* **18**, 211 (2008).
14. Vacancy-induced magnetism in SnO₂: A density functional study
Gul Rahman, Víctor M. García-Suárez, and Soon Cheol Hong, *Phys. Rev. B* **78**, 184404 (2008).
15. Possible magnetism of Be-doped BN nanotubes
Gul Rahman and Soon Cheol Hong, *J. Nanosci. Nanotechnol.* **8**, 4711 (2008).

16. Magnetism of zinc blende Fe chalcogenides: First-principles Calculations
Gul Rahman, Sunghae Cho, and Soon Cheol Hong, *J. Korean. Phys. Soc.* **53**, 380 (2008).
17. Electronic and magnetic properties of digitally Ti doped InP. A first-principles study
Gul Rahman, Sunghae Cho, and Soon Cheol Hong, *Physica Status Solidi (a)* **205**, 1860 (2008).
18. Half metallic ferromagnetism of Mn doped AlSb: A first-principles study
Gul Rahman, Sunghae Cho, and Soon Cheol Hong, *Physica Status Solidi (b)* **244**, 4435 (2007).
19. Magnetism of zinc blende CrP(001) surface.
Gul Rahman, Sunghae Cho, and Soon Cheol Hong, *J. Magn. Magn. Mater.* **310**, 2192 (2007).
20. Magnetic and electronic structures of zinc blende FeX ($X=P, As, Sb$) by first-principles calculations.
Gul Rahman, Sunghae Cho, and Soon Cheol Hong, *J. Magn. Magn. Mater.* **304**, e146 (2006).

ON GOING PROJECTS

1. Magnetism of Ferrous materials
2. Proposing new Diluted magnetic semiconductors (bulk, and nano)
3. Magnetism and Electronic structures of SiC nanoribbons
4. Inducing magnetism in Ferroelectric materials

TALKS AND PRESENTATIONS

1. Ab initio study on magnetism of Al impurity in bcc Fe
Gul Rahman and **In Gee Kim**, IPUSS, Korea, December, 2010,
2. Elastic properties and thermodynamics of bcc Ni_xFe_{1-x} from first-principles
Gul Rahman, **In Gee Kim**, and H.K.D.H. Bhadeshia, KIMS, Autumn meeting Changwon, Korea, November 4, 2010,
3. Magnetism and phase stabilities of Fe-based materials (**Invited**)
Gul Rahman, 35th International Nathiagali Summer College Pakistan, June 28-July 10, 2010.
4. Ferromagnetic-antiferromagnetic transition of CsCl-type FeSe (**Invited**)
Gul Rahman, 35th International Nathiagali Summer College Pakistan, June 28-July 10, 2010.
5. Understanding diluted magnetic semiconductors from first-principles (**Invited**)
Gul Rahman, 35th International Nathiagali Summer College Pakistan, June 28-July 10, 2010.
6. Strain-induced half-metallic ferromagnetism in zinc blende CrP/MnP superlattice (**Invited**)
Gul Rahman, 35th International Nathiagali Summer College Pakistan, June 28-July 10, 2010.
7. A first-principles study on the local magnetic moments of Mn in bcc Fe
Gul Rahman, In Gee Kim, and J. Il Lee, Germany, March (2010).

8. *Ab initio* prediction of pressure-induced structural phase transition of superconducting FeSe(**Invited**)
Gul Rahman, International Scientific Spring ISS-2010, NCP, Islamabad, Pakistan, March (2010).
9. Phase stability of Fe_{16}C_2 and Fe_{16}C_4 from first-principles calculations
Gul Rahman and In Gee Kim, Korean Magnetic Society Meeting, Dec. (2009).
10. Effect of Al impurity on magnetism in bcc Fe by a first-principles calculation
Seung-Woo Seo, **Gul Rahman**, and In Gee Kim, Korean Magnetic Society Meeting, Dec. (2009).
11. Electronic Structure of Ferrite/Cementite Interface: First-principles Study
Gul Rahman and In Gee Kim, International Symposium on Steel and multiscale modeling, September (2009).
12. First-principles prediction of ferromagnetic-antiferromagnetic phase transition of CsCl-type FeSe
Gul Rahman and In Gee Kim, International Conference on Magnetism (ICM), July (2009).
13. Structural phase transitions in FeSe: A first-principles study
Gul Rahman and In Gee Kim, 2nd GIFT-POSCO Joint Industry Meeting, July 03 (2009).
14. Magnetic and electronic structures of Ni impurities in BCC $\text{Fe}_{1-x}\text{Ni}_x$: A first-principles study
Gul Rahman and In Gee Kim, Asia Steel, May (2009).
15. Electronic structures of Bagaryatsky Interfaces: First-principles Study
Gul Rahman and In Gee Kim, International Symposium on Steel and multiscale modeling, December (2008).
16. A first-principles study on magnetic and electronic properties of Ni impurity in BCC Fe
Gul Rahman and In Gee Kim, Asian Magnetism Conference, December (2008).
17. Electronic and magnetic properties of FeSe: A first-principles study
Gul Rahman and In Gee Kim, Korean Physical Society, October (2008).
18. On the phase stability of Fe_{16}C_4 and Fe_{16}C_2
Gul Rahman and In Gee Kim, International Symposium on Steel and multiscale modeling, July (2008).
19. First-principles study on substitutional effects on magnetism in BCC Fe
Gul Rahman, In Gee Kim, and Sam Kyu Chang, Korean Magnetic Society Meeting, June (2008).
20. First principles calculations of half metallic ferromagnetism of zinc blende CrP/MnP superlattice
Gul Rahman, Sunghae Cho, and Soon Cheol Hong, Korean Physical Society Meeting, April (2006).
21. Magnetic and electronic structure of Mn_2As
Gul Rahman, Sunghae Cho, and Soon Cheol Hong, Korean Magnetic Society Meeting, June(2005).
22. Magnetic and electronic structure of Fe_2As by first-principles calculations
Gul Rahman, Sunghae Cho, and Soon Cheol Hong, Korean Physical Society Meeting, October (2005).

23. Metallic antiferromagnetism of zin blende FeX ($X=As,P,Sb,P$) by first-principles calculations
Gul Rahman, Sunglae Cho, and Soon Cheol Hong, Korean Physical Society Meeting, April (2005).
24. Magnetic and electronic structures of FeAs: A first principles calculations
Gul Rahman, Sunglae Cho, and Soon Cheol Hong, Korean Magnetic Society Meeting, December (2004).
25. Magnetic and electronic structures of Mn doped AlSb
Gul Rahman, Sunglae Cho, and Soon Cheol Hong, Korean Physical Society Meeting, October (2004).

INTERNATIONAL
CONFERENCES

1. International Conference on Magnetism, July 2009, Karlsruhe, Germany.
2. International Conference on Asia Steel, May 2009, Pusan, Korea.
3. Asian Magnetics Conference, December 2008, Pusan, Korea.
4. The 13th International Conference on II-VI Compounds, September 2007, Jeju, Korea.
5. Third Seeheim Conference on Magnetism, August 2007, Frankfurt, Germany.
6. 1st International Symposium on Advance Magnetic Materials, June 2007, Jeju Korea.
7. The 18th International Conference on Molecular Electronics and Devices, May 2007, Daejon, Korea.
8. Third Korea-Germany Joint Seminar on Nano Structured Materials, September 2006, Korea.
9. International Conference on Magnetism, August 2006, Kyoto, Japan.
10. The 4th International Conference on Advance Materials and Devices, December 2005, Jeju, Korea.
11. International Symposium on Spintronics and Advance Magnetic Technologies and International Symposium on Magnetic Materials and Applications, August 2005, Taipei, Taiwan.

REFERENCES

On Request