

Talat Shahnaz Rahman

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PROFESSIONAL PREPARATION

1969 B. S. (Honors in Physics), First position graduating class of 1969, University of Karachi, Pakistan
1970 M. Phil (Physics), Islamabad University
1977 Ph.D. (Physics), University of Rochester; *Advisor: R.S. Knox*
1977-1979 Postdoctoral Associate, University of California, Irvine; *Mentors: D.L. Mills & A.A. Maradudin*

APPOINTMENTS

2012 - Pegasus Professor, Department of Physics, University of Central Florida
2015 - Co-leader, UCF Faculty Cluster on Rational Design of Catalysts for Energy Applications
2006 - Distinguished Professor, Department of Physics, University of Central Florida
2006 - 2015 Chair, Department of Physics, University of Central Florida
2001 - 2006 University Distinguished Professor, Kansas State University
1991 - 2001 Professor, Kansas State University
1986 - 1991 Associate Professor, Kansas State University
1983 - 1986 Assistant Professor, Kansas State University
1979 - 1982 Assistant Research Physicist, University of California, Irvine

VISITING APPOINTMENTS

Miller Visiting Professor, University of California Berkeley, Spring Semester, 2018
Visiting Scientist, Aalto University, Espoo, Finland, March-June, 2017; December, 2017
Visiting Scientist, Donostia International Physics Center, San Sebastian, Dec. 2016 - Feb. 2017; July 2017
Visiting Scientist, Max Planck Institut für Festkörperforschung, Stuttgart, July, 2009-2015, Aug-Oct. 2016
Visiting Scientist, Fritz Haber Institut der MPG, Berlin, Summer 1998-2007; Spring 2001
Visiting University Professor, Helsinki University of Technology, Finland, Aug. 2000 – Jan. 2001
Adjunct Professor, National Center for Physics, Islamabad, Pakistan, 2004 – 2009
Visiting Scientist, Max Planck Institut für Strömungsforschung, Göttingen, June-July, 1997
Visiting Scientist, Freie Universität Berlin and Fritz Haber Institute, Berlin, July-August, 1996
Professor Invité, Ecole Polytechnique Federal de Lausanne, Lausanne, Switzerland, June-August 1993
Visiting Physicist, Brookhaven National Laboratory, Sept. 1992-May 1993
Visiting Scientist, Sandia Laboratories, Livermore, July-Sept. 1992
Guest Scientist, Forschungszentrum, Jülich, July 1991, Summer Months 1984-89
Faculty Research Participant, Argonne National Lab., May-August 1990; June-August 1995
Research Physicist, University of California, Irvine, May-August 1983

SELECTED FELLOWSHIPS, AWARDS, & HONORS

2017 Miller Visiting Professorship, University of California, Berkeley
2017 Research Incentive Award, University of Central Florida
2017 Excellence in Research Award, College of Sciences, University of Central Florida
2017 Member, Committee on Frontiers of Materials Research: A Decadal Survey, National Academies
2017 Appointed to the Physical Sciences Advisory Board, Oak Ridge National Laboratory
2017 Founding Section Editor, Journal of Physics Condensed Matter

2016 Fellow, American Vacuum Society (AVS)
2016 Chair, APS Topical Group on Energy Research and Applications (GERA)
2016 Chair, Davisson and Germer Prize Committee, American Physical Society
2016 Editorial Board Member, Progress in Surface Science
2015 Vice Chair, Davisson and Germer Prize Committee, American Physical Society
2012 ORC Millionaires Club, 2012-13, University of Central Florida
2012 Pegasus Professor, University of Central Florida
2011 Research Incentive Award, University of Central Florida
2011 University of Central Florida - ORC Millionaires Club, 2011-12
2007 Sigma Pi Sigma Member, Honorary Member, UCF
2004 Sigma-Xi Distinguished Lecturer (2004-2006)
2003 Phi Beta Kappa, Honorary Member, Beta Chapter, KSU
2002 Higuchi Research Achievement Award (Olin K. Petefish Prize), University of Kansas
2001 University Distinguished Professor, Kansas State University
2000 Alexander von Humboldt Research Prize, Germany
1998 Distinguished Graduate Faculty Award, Kansas State University
1998 Fellow, American Physical Society
1994 UNDP-TOKTEN Fellowship, Quaid-e-Azam University, Islamabad, Pakistan
1993 CNRS-Italy Fellowship
1992 Stamey Undergraduate Teaching Award, Kansas State University
1987 Alexander von Humboldt Research Fellowship, Germany, 1987-88

SCIENTIFIC PRODUCTIVITY

Publications: over 260 in refereed high impact journals (full list attached). *Citations:* 7896; *h-index:* 50

<https://scholar.google.com/citations?user=tel1v6oAAAAJ&hl=en&oi=ao>

Invited Presentations: on average about 12 – 20 invited talks per year.

PRINCIPAL RESEARCH TOPICS

Multi-scale modeling of chemical reactions and related phenomena at surfaces
Understanding processes that control growth and morphological evolution of thin films
Theory and modeling of vibrational, optical and magnetic properties of nanomaterials
Predictive modeling of functional two-dimensional transition metal dichalcogenides
Surface coordination chemistry: novel functionality via substrate charge transfer and oxidation state
Understanding the response of surfaces and nanostructures to ultrafast external fields
Development of techniques beyond density functional theory for strongly correlated materials
Development of techniques suitable for non-equilibrium phenomena and non-adiabatic processes
Rational designing of quantum materials

MEMBERSHIPS

- APS (American Physical Society)
- ACS (American Chemical Society)
- AVS (American Vacuum Society)
- AAPT (American Association of Physics Teachers)
- AAAS (American Association for the Advancement of Science)
- MRS (Materials Research Society)
- PhysTEC (Physics Teachers Education Coalition): aimed at increasing number of physics teachers)
- APS Bridge Program (aimed at increasing number of physics PhDs from underrepresented groups)

- National Mentoring Community established 2015 by American Physical Society

CURRENT FUNDED PROJECTS

- DOE: DE-FG02-07ER15842 “Controlling Structural, Electronic, and Energy Flow Dynamics of Catalytic Processes through Tailored Nanostructures” (2003 - present) (Co-PIs: Bartels & Dowben)
- DOE: DE-FG02-07ER46354 “Theoretical and Computational Studies of Functional Nanoalloys and other Nanomaterials” (1993 - present)
- NSF: MMN 1710306 “Collaborative Research- Connecting Mesoscale Dynamics of Metallic Films on Semiconductors to Nanoscale Phenomena,” (9/1/2017 – 8/31/2020)
- NSF: CHE-1465105 “SusChEM Defect-laden 2D Catalysts for Carbon Sequestration and Safer Hydrogenation” (2015-2018) (PI: Richard Blair, Co-PI: Laurene Tetard)
- NSF: DUE-1246024 “Active Learning Strategies for Algebra-based Introductory Physics Courses at UCF” (2013-17) (Co-PIs: Chini, Kara, Flytsiyan, Dubey)
- APS Site Grant: “UCF PhysTEC Comprehensive Site,” (2013-2016); locally sustained till 2019 (with UCF Physics team).
- APS Site Grant: “UCF APS-Bridge Program Site” (2015-2018); locally sustained till 2021 (with UCF Physics team).
- NSF: CHE-1310327 “Surface Coordination Chemistry: Toward Novel Functionality” (2013-17)
- NSF: INT-1134698 “US-Pakistan Workshop: International Nathiagali Summer College” (2011-2017)

EXTERNAL RESEARCH FUNDING at UCF (2006-present): \$7,988,866

LANGUAGES SPOKEN

Fluent in English, Urdu, Hindi and Bengali; comfortable in German, broken in French.

GRADUATE STUDENTS SUPERVISED

Jin He, Ph.D., 1987	Duy Tran The Le, PhD, 2012
Liqui Yang, Ph.D., 1991	Maral Aminpour, PhD, 2013
Kai Yang, Ph.D., 1991	Syed Islamuddin, PhD, 2013
Wes Bailey, Masters, 1995	Neha Nayyar, PhD, 2014
Pavlin Staikov, Ph.D., 1998	Alamgir Kabir, PhD, 2015
Sondan Durukanolgu, Ph.D., 1999	Ghazal Shafai, PhD, 2016
Ahlam Al-Rawi, Ph.D., 2000	Jarrad Pond, PhD 2016
Weibin Fei, Ph.D., 2000	Takat Rawal, PhD 2017
Chandana Ghosh, PhD, 2003	Shree-Ram Acharya, PhD 2018
Sampyo Hong, PhD, 2005	Zahra Hooshmand, PhD in progress
Faisal Mehmood, PhD, 2006	Nasim Uddin, PhD in progress
Altaf Karim, PhD, 2006	Tao Jiang, PhD in progress
Marisol Alcantar Ortegoza, PhD, 2007	Mahboob ur Rehman, PhD in progress
Handan Yildirim, PhD, 2010	Andre Childs, pre-candidacy

POST-DOCTORAL ADVISEES AND RESEACH ASSOCIATES

Dr. Sergey Stolbov, 2000 - 2007	Dr. Alfredo Ramirez, 2012 – 2014
Dr. Zengju Tian, 1993	Dr. Volodymyr Turkowski, 2008 – present
Dr. Abdelkader Kara, 1994 – 2007	Dr. Marisol Alacantara Ortegoza, 2008 – 2012

Dr. Ulrike Kürpick, 1995-98	Dr. Giridhar Nandipati, 2009 – 2012
Dr. Ahlam Al-Rawi, 2003- 2009	Dr. Sampyo Hong, 2005 – 2014
Dr. Vasse Chis, 2009 – 2010	Dr. Duy Le, 2012 – present
Dr. Chandana Ghosh, 2008- 2011	Dr. Jacquelyn Chini, 2010 - 2013

UNIVERSITY SERVICE

At University of Central Florida:

Faculty Compliance Advisory Committee, 2017
 Promotion and Tenure Committee, UCF Research Centers 2016-2018
 Search Committee Chair for Chair of UCF Chemistry Department, 2015
 Adhoc Committee for Undergraduate Program, College of Optics and Photonics, 2014 -
 Search Committee for Director of NanoScience and Technology Center and AMPAC, 2009
 Search Committee for Dean of the College of Optics and Photonic, 2008
 Search Committee for Dean of the College of Science, 2007
 Promotion and Tenure Committee, NSTC, 2006-2008
 Served/serving on many Graduate Student PhD Committees in Physics, Chemistry and CREOL
 Mentor to a large number of female faculty members & students at both KSU and UCF
 Faculty Compliance Advisory Committee, 2017 -

At Kansan State University:

President-Elect, President, Past-President, KSU Faculty Senate, 1997-2000
 Faculty Senate Executive Committee 1991-92, 1997-2000
 Faculty Senate Committee on University Planning, 1999-2000
 Faculty Senator 1990-92, 1993-2000, 2001-present
 Faculty Affairs Committee of the Faculty Senate 1994-95
 Chair, KSU's Developing Scholar Program, 2000
 University Strategic Planning Committee, 1999
 Chair, Task Force on Enhancing Retention and Graduation Rates for Minority Students, 1999-00
 Task Force on Appeal and Grievance Procedures, 1997-98; Task Force on Equity Issues, 1999-00
 Dean of Arts and Sciences' Review Committee 1995
 Adhoc Committee on International Activities Center 1995-1998
 Kansas Computer Planning Committee--KSTAR/NSF EPSCoR 1995-97
 Task Force on High Performance Supercomputing, 1998-99
 Selection Committee for Sloan Mentoring Fellowships 1994-96
 Search Committee for Theoretical Bio-Chemist, 1996; Theoretical Chemist, 1996
 Search Committee for Co-Director Affirmative Action 1996
 Common University Degree Requirement Committee 1988-90
 Member International Activities Council, 1989-92
 President's Commission on Multicultural Affairs 1990-present
 Search Committee for Dean, College of Arts and Sciences, 2002-03
 Presidential Lecturer 1990-1999
 Director, Center for Scientific Supercomputing, 1997-2000
 Served on numerous Departmental Committees and Graduate Student PhD Committees

PROFESSIONAL SERVICE AT THE NATIONAL LEVEL (selected examples):

- Member, Physical Sciences Advisory Board, Oak Ridge National Laboratory, 2017-2020
- Member, Committee on Frontiers of Materials Research: A Decadal Survey, National Academies of Sciences, Engineering and Medicine, March 2017 – August 2018.

- Scientific Advisor, NOVA science program, Public Broadcasting Service, 2006 –.
- Physics Department Program Reviewer:
 - a) University of North Florida 2009;
 - b) University of North Carolina, Charlotte, 2015;
 - c) University of Kansas, 2016.

PROFESSIONAL SERVICE AT THE NATIONAL LEVEL (continued):

For US Department of Energy and National Science Foundation:

- Regularly asked to serve on DOE-BES panel reviews. Recent panels include:
 - INCITE Material Science initiative, 2011 (panel Chair), 2012 (panel Chair)
 - INCITE Material Science initiative, 2009, 2010 (panel Member)
 - Program Review, Material Science Division, Lawrence Berkeley, 2012
 - Computational Material Science Network program, April 19-20, 2010
 - Energy Frontier Research Centers Initiative, February 23-25, 2009.
 - Theory, Modeling and Simulation (TMS) Panel Review April 20-21, 2009.
 - BES Division, Oak Ridge National Laboratory, January 2006.
 - SUNCAT Research Center, Stanford University/SLAC, April 2016.
 - BES Division, Energy Frontier Research Center mid-term review, February 2016.
- Served as reviewer for several recent high profile initiatives:
 - DOE Office of Science Graduate Fellowship Program (DOE SCGF) 2009, 2011, 2012
 - DOE Catalysis Science Early Career Proposals, 2009-2015, 2018
- Invited by DOE to serve on its Scientific Organizing Committee for Computational Materials Science Network, 2009-11.
- Invited participant, DOE-BES/ASCR Extreme Scale Workshop, August 12-15, 2009.
- Committee of Visitors, Division of Materials Research, National Science Foundation, 2008.
- Moderator, DOE panel on Future Directions in Computational Nanocatalysis, Center for Functional Nanomaterials, Brookhaven National Laboratory, Tarrytown, October 19-21, 2005.
- Participant in several site visits for research Center proposals to NSF and DOE
- Very frequent reviewer of research proposals from a large number of federal agencies
- Ongoing evaluation panel member for NSF funding initiatives such as NIRT, IGERT, MRI, CDI, MRSEC, DMREF

For American Physical Society:

- Vice Chair (2014), Chair-Elect (2015), Chair (2016) Topical Group on Energy Research and Applications (GERA)
- Member PhysTEC Site visit team, Georgia State University, Atlanta, April 3, 2014
- Member PhysTEC Site visit team, University of Alabama, March 23, 2015
- Executive Committee, Division of Materials Physics, American Physical Society, 2002-2005
- APS site visit team for “Improving the climate for women” in Physics departments, 2004 -2005.
- Nominating Committee Member, Forum on International Physics, 2009 -2011
- Co-organizer, Focused Session on "Computational Design of Novel Materials," APS March Meeting 2010, Portland.
- Co-organizer, Focused Session on "van der Waals Bonding in Advance Materials," APS March Meeting 2012, Boston.
- Co-organizer Focused Session on "Computational Nanoscience," APS March Meeting 2007, Denver.
- Co-organizer, Focused Session on "Computer Simulations of Complex Materials," APS March Meeting 2004, Montreal.

- Co-organizer, Focused Session on "Surfaces, Interfaces and Growth of Thin Films," APS March Meeting 2001, Seattle.
- Co-organizer Focused Session on "Computational Nanoscience," APS March Meeting 2005, Los Angeles.

For American Vacuum Society:

- Chair, Diversity and Inclusion Sub-Committee (within Committee for Education)
- Member, National Multi-society Diversity Committee
- Executive Committee Member, American Vacuum Society, Surface Science Division, 2014-2016.
- Program Chair, Focus Topic: Accelerating Materials Discovery for Global Competitiveness, 62nd AVS International Symposium & Exhibit, San Jose, October (2015).
- Program Committee Member, Focus Topic: Accelerating Materials Discovery for Global Competitiveness, 61st AVS International Symposium & Exhibit, Long Beach, October (2014).

PROFESSIONAL CONTRIBUTIONS AT THE INTERNATIONAL LEVEL (selected examples)

Funding Agencies and Academic Institutions

- One of three international experts invited to advise Physics Department Faculty Hiring Committee, Tampere University, Finland, on tenure-track faculty candidates, April 2018.
- One of three international experts invited to advise University of Gothenburg, Sweden, on the establishment of a Marine Sciences Department, October 2014.
- Chair, Review Panel for Physics and Mathematics Departments, University of Gothenburg, Sweden, 2010-11.
- Review Panel Member for Villanova Research Foundation, Government of Sweden, for selection of Centers of Excellence in Materials, May-September, 2009
- Vice Chair, Scientific Review Panel for Physics and Mathematics Departments, Lund University, Sweden, 2007- 2008.
- One of two experts in the hiring committee for a faculty position in Theoretical Chemical Physics, Stockholm University, Sweden, 2008
- Member International Evaluation Committee for Condensed Matter Physics Research in Sweden, Swedish Research Council, 2004 - 2005.
- Regular reviewer of research proposals for funding agencies such as International Science Foundation, National Research Council of Hong Kong, Swedish Research Council, International Center for Theoretical Physics (Trieste), Czech Research Foundation, etc..
- Adjunct Professor, National Center for Physics, Islamabad, Pakistan, 2005 –
- Serving as consultant to the Coordinator General (Dr. Shaukat Hameed) of COMSTECH, the Ministerial Standing Committee on Scientific and Technological Cooperation of the Organization of Islamic Cooperation, 2014 - .
- Scientific Advisory Board, Lahore University of Management Science, Lahore, Pakistan, 2009 –
- Member, Board of Directors, GIK Institute of Technology, Topi, Pakistan, 2004-2006.
- "Opponent" (external examiner) for the thesis defense of:
 - a. T. Hjelt, Helsinki Institute of Technology, Helsinki, Finland, November, 1999.
 - b. Karin Carlin, Chalmers Institute of Technology, Goteborg, Sweden, May, 2003.
 - c. Aleksandra Vojvodic, Chalmers Institute of Technology, Goteborg, December, 2009.
 - d. Andris Gulens, Department of Applied Physics, Aalto University, Finland, January 2012.
- Served as examiner of Ph.D. thesis of:
 - a. Dr. Ilpo Vattulainen, Helsinki Institute of Technology, Finland, November 1997.
 - b. Dr. Zakir Hussain, Bahawalpur University, Pakistan, 2016
 - c. Dr. Waqas Hussain, COMSATS Institute of Technology, 2012.

Scientific Journal Editorial Boards:

- Editorial Executive Board Member, Journal of Physics: Condensed Matter, IOP, 2009 – present
- Founding Section Editor, Physics of Chemical Processes, Journal of Physics: Condensed Matter, IOP, 2017 – present
- Editorial Advisory Board Member, Journal of Physics: Condensed Matter, IOP, 2006 – 2009.
- Editorial Board Member, Journal of Theoretical and Computational Nanoscience, 2003 – 2006.
- Guest Editor, Special Issue “Computational Techniques for Designing Materials,” Journal of Physics: Condensed Matter, Volume 21, No. 8, 2009
- Guest Editor, Special Issue “van der Waals Bonding in Advanced Materials,” Journal of Physics: Condensed Matter, Volume 24, July 2012.

Conferences and Workshops

- Member, International Organizing Committee, International Conference on Solid Films and Surfaces 2012-present.
- Member, International Organizing Committee, European Conference on Surface Science, 2008-2011.
- Advisory Board Member, 17th International Conference on Solid Films and Surfaces, July, 2014, Rio de Janeiro, Brazil.
- Advisory Board Member, 16th International Conference on Solid Films and Surfaces, 1-6 July, 2012, Genoa, Italy.
- International Organizing Committee, biannual meetings on Vibrations at Surfaces (VAS).
- Organizer of week-long condensed matter physics program at International Nathiagali Summer College (INSC) held annually at Nathiagali, Pakistan (I am also responsible for selecting US participant whose travel expenses have been funded through an NSF grant awarded), 1998-2012.
- Through INSCs, follow-up workshops, and scientific visits, continue to help establish and strengthen several prominent research groups in Pakistan, most requiring negotiations with government officials.
- Organizer, 13th International Conference on Vibrations at Surfaces, Orlando, Florida, March 10-13, 2010).
- Organizer of series of workshops on computational material design, Islamabad, Pakistan (with local institutions: NCP, COMSTECH, COMSATS Institute of Information Technology), 2001 – present.
- Chair, 13th International Conference on Vibrations at Surfaces, Orlando, March 10-13, 2010.
- Organizing Committee for Workshop “Atomistic and mesoscale modeling of materials defects,” Oct. 22-26, 2012, Los Angeles, Institute for Pure and Applied Mathematics (IPAM).
- Invited as a long term core participant to IPAM’s 14 week program, Materials Defects: Mathematics, Computation, and Engineering”, September 10 to December 14, 2012.
- Organizing Committee, 11th International Conference on Vibrations at Surfaces, June 6-10, 2004, Maine.
- Co-organizer, 11th International Workshop on Surface Dynamics, Rolla, Missouri, Oct. 4-6, 2003.
- Co-organizer, 10th International Workshop on Surface Dynamics, El Escorial, Spain, June, 2001.
- Presented Workshop on "Annual and Post-Tenure Reviews in the Light of Scholarship Reconsidered" with Provost J. Coffman and Dr. B. Fenwick, Eighth AAHE Conference on Faculty Roles and Rewards, New Orleans, February 3-6, 2000.
- Presented Workshop on "Annual, Tenure, and Post-Tenure Reviews: Balancing Process, Productivity, and Perceptions" with Provost J. Coffman and Dr. B. Fenwick, Seventh AAHE Conference on Faculty Roles and Rewards, San Diego, January 21-24, 1999.

- Chair, 9th International Workshop on Surface Dynamics, Charlottesville, Virginia, June, 1999.
- Organizer, 23rd Midwest Solid State Theory Symposium, Manhattan, Kansas, October, 1995.
- International Organizing Committee, biannual meetings on Vibrations at Surfaces (VAS) 1995 –

PROFESSIONAL CONTRIBUTIONS AIMED AT WOMEN & MINORITIES (selected examples):

- Helped establish in 2012 the Women in Physics Group (WPG) at UCF, which continues to be active: organizes monthly networking events and arranges mentoring and outreach activities to recruit and retain young women in STEM disciplines.
- Together with WPG, facilitated the organization of the 2013 Southeastern Conference for Undergraduate Women in Physics at UCF. About 120 women engaged in an exciting workshop with 18 successful female physicists.
- As site leader of the APS Bridge Program grant (3 year APS + 3 year UCF commitment), engaged in establishing policies and procedures that help recruit and retain physics graduate students from underrepresented minority (URM) groups. Twelve students admitted 2014-16. At least 4 to be admitted per year for the next five years.
- Invited to Virginia Tech University, May 3-5, 2016, to advise faculty and administrators on strategies that help recruit and retain URM students.
- As the first female physics faculty member at Kansas State University, helped create a female friendly environment, leading to increased numbers of female graduate students and faculty in the period 1984-2006.
- Served formally as faculty mentor at Kansas State University to several female faculty members, as part of a Sloan Foundation Grant (1993-1995). These faculty members are successful professionals.
- Worked with Committee on the Status of Women in Physics, American Physical Society, in its efforts to change the climate for women and minorities through Site visits.
- As President of Faculty Senate at Kansas State University, 1998-99, initiated a process for system-wide study of gender equity issues in all Kansas universities, endorsed by the Kansas Board of Regents. A large number of equity issues were resolved as a consequence.
- As chair of the Task Force on Enhancing Retention and Graduation Rates for Minority Students, 1999-2000, helped establish a program at Kansas State University (Developing Scholars), which continues to be successful at recruiting and retaining students from historically underrepresented groups.
- As KSU Presidential Lecturer 1990-1999, served as a frequent speaker at K-12 institutions in Kansas, with the aim of recruiting women and minorities to STEM disciplines.
- As a member of the Faculty Senate Executive Committee, KSU, 1991-92, 1997-2000, helped introduce policies regarding tenure-clock stoppage and maternity leave for better retention of female faculty members.
- As author of the article “Should we tell our daughters to become scientists?” CSWP Gazette, 24, 3 (2005), invited to present Sigma Xi Distinguished Lecture at a number of US academic institutions.
- Survey of Career Satisfaction of Senior US Women Physicist, conducted in collaboration with Kathy Levin, University of Chicago and Rachel Ivey, American Institute of Physics, 2006.
- Following the Survey of Career Satisfaction of Senior US Women Physicists, organized a NSF-ADVANCE Workshop: Women in Science and Engineering at Kansas State University, February 15-16, 2008.
- Wrote a solicited article “Should we tell our daughters to become scientist?” CSWP Gazette, 24, 3 (2005), which was based on several talks that I had given on the topic as a Sigma Xi Distinguished Lecturer. The article points to some ways in which young girls can overcome hurdles and get excited about scientific careers at an early age.
- As chair of the UCF Physics Department (2006 – 2015), encouraged policies and programs that help create a female-friendly environment, as signified by a noticeable increase in the number of female students and faculty members; initiated a lactation room in the new Physical Sciences building.

- Helped establish a program at Kansas State University (Developing Scholars), 1999-2000 aimed at recruiting and retaining students from historically underrepresented groups. The program continues to thrive and achieve its goals.
- Engaged in STEM related activities with teachers in the Orlando area K-12 institutions, 2009 -

PROFESSIONAL CONTRIBUTIONS AIMED AT REFORMING STEM EDUCATION

- As the PI of the APS PhysTEC Comprehensive Site grant, 2013 – present, engaged in recruitment and training of physics majors as future science teachers to address the shortage of teachers with sound content knowledge. In this regard also helped establish a teacher-in-residence program which in turn strengthened the interaction with local high school teachers.
- In 2011, I helped establish a successful Learning Assistant (LA) program in the Physics Department at UCF, based on the University of Boulder model, which emphasizes peer-instruction through pedagogical training of the undergraduates who serve as LAs.
- I am leading NSF-supported pedagogy reform in introductory physics courses via active learning environment (studio) and inquiry-based methodology. I have also facilitated such reforms in upper-division physics courses.

PUBLICATIONS

1. S. R. Acharya and T. S. **Rahman**, “Towards Multiscale Modeling of Thin Film Growth Processes using SLKMC,” *J. Mat. Res.* 33, 709 (2018).
2. K. Kuhnke, V. Turkowski, A. Kabakchiev, T. Lutz, T. S. **Rahman**, and K. Kern, “Properties of pentacene excitons in strong electric fields,” *ChemPhysChem* 19, 277 (2018).
3. C. D. Tempas, T.W. Morris, D. L. Wisman, N U. Din, D. Le, B. J. Cook, A. V. Polezhaev, T. S. **Rahman**, K. G. Caulton, and S. L. Tait, “Redox-active Ligand Controlled Selectivity of Vanadium Oxidation on Au(100),” *Chem. Sci.* 9, 1674 (2018).
4. C.S. Merida, D. Le, E.M. Echeverria, A.E. Nguyen, T.B. Rawal, S.N. Alvillar, V. Kandyba, A. Al-Mahboob, Y. Losovyj, K. Katsiev, M.D. Valentin, C.-Y. Huang, M.J. Gomez, I.-H. Lu, A. Guan, A. Barinov, T.S. **Rahman**, P.A. Dowben, and L. Bartels, "Gold Dispersion and Activation on the Basal Plane of Single-Layer MoS₂," *J. Phys. Chem. C* 122, 267 (2018).
5. P. E. Evans, H. K. Jeong, Z. Hooshmand, D. Le, T. B. Rawal, S. N. Alvillar, L. Bartels, T. S. **Rahman**, and P. A. Dowben, “Methoxy Formation Induced Defects on MoS₂,” *J. Phys. Chem. C* (Just Accepted) DOI: 10.1021/acs.jpcc.8b02053
6. S. Rauschenbach, G. Rinke, R. Gutzler, S. Abb, A. Albargash, D. Le, T. S. **Rahman**, M. Durr, L. Harnau, and K. Kern, "Two-Dimensional Folding of Polypeptides into Molecular Nanostructures," *ACS Nano* 11, 2420 (2017).
7. S. R. Acharya, S. I. Shah, and T.S. **Rahman**, “Diffusion of Small Cu Islands on the Ni(111) Surface A self-learning kinetic Monte Carlo study,” *Surface Science*, 662, 42 (2017).
8. T. B. Rawal, D. Le, and T. S. **Rahman**, “Effect of single-layer MoS₂ on the geometry, electronic structure, and reactivity of transition metal nanoparticles,” *J. Phys. Chem. C* 121, 7282 (2017).
9. D. Le and T. S. **Rahman**, “Pt-Dipyridyl Tetrazine metal-organic network on the Au(100) surface: Insights from first principles calculations,” *Faraday Transactions* 204, 83 (2017) DOI: 10.1039/C7FD00097A.
10. A. Gupta, T. B. Rawal, C. J. Neal, S. Das, T. S. **Rahman**, and S. Seal, “Molybdenum Disulfide for Ultra-Low Detection of Free Radicals: Electrochemical Response and Molecular Modeling,” *2D Materials* 4, 025077 (2017).

11. J. Pal, T. B. Rawal, M. Smerieri, S. Hong, M. Alatalo, L. Savio, L. Vattuone, T. S. **Rahman**, and M. Rocca, "Adatom extraction off pristine terraces by dissociative oxygen adsorption at metal surfaces: Combined STM and DFT investigation of O/Ag(110)," *Phys. Rev. Lett.* 118, 226101 (2017).
12. Z. Hooshmand, D. Le, and T.S. **Rahman**, "CO Adsorption on Pd(111) at 0.5ML: A First Principles Study," *Surf. Sci.* 655, 7-11 (2017).
13. T. Komesua, D. Le, I. Tanabe, E. F. Schwier, Y. Kojima, M. Zheng, K. Taguchi, K. Miyamoto, T. Okuda, H. Iwasawa, K. Shimada, T. S. **Rahman**, and P. A. Dowben, "Adsorbate doping of MoS₂ and WSe₂: the influence of Na and Co," *J. Phys. Condens. Matter.* 29, 285501 (2017).
14. T.B. Rawal, D. Le, and T.S. **Rahman**, "MoS₂-Supported Gold Nanoparticle for CO Hydrogenation," *J. Phys.: Condens. Matter* 29 415201 (2017).
15. V. Turkowski and T.S. **Rahman**, "Nonadiabatic exchange-correlation kernel for strongly correlated materials," *Journal of Physics: Condensed Matter* 29, 455601 (2017).
16. V. Turkowski, N. Uddin and T. S. **Rahman**, "Time-Dependent Density-Functional Theory and Excitons in Bulk and Two-Dimensional Semiconductors," *Computations* 5, 39 (2017).
17. P. Patoka, G. Ulrich, A.E. Nguyen, L. Bartels, P.A. Dowben, V. Turkowski, **T.S. Rahman**, P. Hermann, B. Kästner, A. Hoehl, G. Ulm, and E. Rühl, "Nanoscale plasmonic phenomena in CVD-grown MoS₂ monolayer revealed by ultra-broadband synchrotron radiation based nano-FTIR spectroscopy and near-field microscopy", *Optics Express* 24, 1154 (2016).
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INVITED TALKS (2000 – present)

2018

1. “Manipulating properties of 2D materials: old stuff with new promises,” Condensed Matter Physics Seminar, University of California, Davis, April 26, 2018.
2. “Multiple excitations, excited states, and ultrafast charge dynamics of functional materials: insights from TDDFT+DMFT,” Molecular Foundry Seminar, Lawrence Berkeley National Laboratory, April 20, 2018.
3. “Tuning 2D materials MoS₂ and h-BN for hydrogenation reactions,” 255th Annual ACS Meeting, New Orleans, March 18-22, 2018.
4. “Supported Au nanoparticles: good for methanol decomposition or formation?” American Physical Society March Meeting, Los Angeles, March 5-8, 2018.
5. “2D Materials: old stuff, new promises, and my Miller time,” Miller Institute Lunch Talk, University of California Berkeley, February 27, 2018.
6. “Nanomaterial pursuit 2018: Inclusive or exclusive?” 2018 Conference for Undergraduate Women in Physics, University of North Florida, January 12-14, 2018

2017

7. “Towards multi-scale modeling of thin film growth processes,” Fall Meeting of Materials Research Society (MRS), Boston, Nov. 26 – Dec. 1, 2017.
8. “Tailoring Chemical & Optical Properties of 2D Materials,” Chemical Physics Department Annual Workshop, Fritz Haber Institute, Doellensee, September 25-29, 2017.
9. “Rational Material Design for Energy Needs: theory and experiment working in tandem,” Karachi University, August 30, 2017
10. “Rational Material Design for Energy Needs: Follow up Workshop, COMSATS Institute for Information Technology, Islamabad, August 29, 2017
11. “Manipulating Chemical Reactivity of MoS₂ and other 2D Materials,” Telluride Workshop on Computational Chemistry, August 7-11, 2017, Telluride.
12. “Pt-Dipyridyl Tetrazine metal-organic network on Au(100): Insights from first principles calculations,” Faraday Society Discussions on Complex Molecular Surfaces and Interfaces, Sheffield, UK, July 24-26, 2017.
13. “2D Transition Metal Dichalcogenides: old materials with new promises,” Gesellschaft Deutscher Chemiker (GdCH) Colloquium, Ruhr University Bochum, July 6, 2017.
14. “Tailoring optical & chemical properties of 2D transition metal dichalcogenides,” Summer School on Surfaces & Interfaces, San Sebastian, June 19-23, 2017.
15. “2D Transition Metal Dichalcogenides: old materials with new promises,” Center for Nanoscience, Universitat Autònoma Barcelona, June 16, 2017.
16. “Rational Design of Functional Nanomaterials : Theory and Experiment working in Tandem,” (2 invited lectures), Workshop on Rational Material Design, COMSTECH, Islamabad, May 22-26, 2017.
17. “Tuning chemical reactivity of MoS₂ and other 2D materials,” Department of Chemistry and Chemical Engineering Seminar, Aalto University, Finland, May 15, 2017.
18. “Rational Designing of Chemical & Optical Properties of 2D Transition Metal Dichalcogenides,” COMP Seminar, Department of Applied Physics, Aalto University, Finland, April 19, 2017

19. “Computational Design of Metal –Coordination Centers for Catalytic Applications,” 253rd ACS Spring Meeting, San Francisco, April 2-6, 2017.
20. “Tailoring properties of 2D transition metal dichalcogenides: looking beyond graphene,” TMS Annual Meeting, San Diego, February 26-March 2, 2017.
21. “Graduate program assessment,” Graduate Education & APS Bridge Program Conference, College Park, Maryland, February 10-12, 2017 (panelist).
22. “Cultivating relationships with School of Education,” PhysTEC Annual Meeting, Atlanta, February 16-18, 2017 (panelist).
23. “Rational design of functional 2D materials,” Donostia International Physics Center, San Sebastian, Spain, January 9-31, 2017 (5 lectures).

2016

24. “Tailoring chemical and optical properties of 2D transition metal dichalcogenides,” 2nd NOOR International Symposium on Applied Materials and Devices,” Nilope, Pakistan, November 14-16, 2016.
25. “On computational design of functional 2D transition metal dichalcogenides,” Max Planck Institute Workshop (Abteilung Kern), Schloss Ringberg, Taegernsee, October 16-19, 2016.
26. “Tailoring properties of 2D transition metal dichalcogenides: looking beyond graphene,” IX International Conference on Surface, Materials and Vacuum, Mazatlán, September 26-30, 2016. (plenary talk)
27. “Time-Dependent Density-Functional Theory with Dynamical Mean-Field Theory: towards ab initio tools for strongly correlated system,” IX International Conference on Surface, Materials and Vacuum, Mazatlán, September 26-30, 2016.
28. “Passion for science,” Materials Science Colloquium, University of Milan, Bicocca, Italy, September 22, 2016.
29. “Tailoring chemical and optical properties of 2D transition metal dichalcogenides,” International Conference on Solid Films and Surfaces (ICSFS18), Chemnitz, August 28-September 2, 2016.
30. “Time-Dependent Density-Functional Theory with Dynamical Mean-Field Theory: towards ab initio tools for strongly correlated and/or out-of-equilibrium systems,” DOE, Theoretical Condensed Matter Physics PIs Meeting, Gaithersburg, August 14-17, 2016.
31. “Reaction mechanisms: interplay of thermodynamics and kinetics,” 2016 DOE Catalysis Science PIs Meeting, Gaithersburg, June 21-24, 2016.
32. “Controlling structural, electronic, and energy flow dynamics of catalytic processes through tailored nanostructures,” DOE-EERE 2016 Annual Merit Review Meeting, Washington, DC, June 6-8, 2016 (invited poster).
33. “Tailoring properties of 2D transition metal dichalcogenides: looking beyond graphene,” Physics Colloquium, Oulu University, Finland, June 3, 2016.
34. “Tailoring chemical properties of single and bilayer layer transition metal dichalcogenides,” Atomic structure of nanosystems from first-principles simulations and microscopy experiments (AS-SIMEX 2016), Physics Boat Series, Helsinki-Stockholm, May 31 – June 2, 2016.
35. “Tailoring Characteristics of Nanoparticles: size, shape, composition and environment matters,” Institute of Physics Seminar, Aalto University, May 30, 2016.
36. “Can an everyday lubricant be a novel material?” Physics seminar, University of the West Indies, Barbados, May 13, 2016.

37. "Can an everyday lubricant be a novel material?" Condensed Matter Physics seminar, Virginia Tech University, May 4, 2016.
38. "Towards increasing diversity in the UCF Physics Department: course reforms and the APS Bridge Program," Virginia Tech University, May 4, 2016.
39. "Active learning strategies for algebra based introductory physics courses UCF," NSF-AAAS Conference, Envisioning the Future of Undergraduate STEM Education (EnFUSE): Research and Practice, April 27-29, 2016, Washington, DC.
40. "Tailoring properties of single and bilayer layer transition metal dichalcogenides: looking beyond graphene," Texas State University Physics seminar, April 12, 2016.
41. "Tailoring properties of single and bilayer layer transition metal dichalcogenides: looking beyond graphene," Joint Spring 2016 Meeting of the Texas Sections of APS, AAPT, and Zone 13 of SPS, March 31 - April 2, 2016, Lamar University, Beaumont, Texas.
42. "A glimpse at the workings of PhysTEC Comprehensive Site and APS Bridge Program Site at UCF," Joint Spring 2016 Meeting of the Texas Sections of APS, AAPT, and Zone 13 of SPS, March 31 - April 2, 2016, Lamar University, Beaumont, Texas.
43. "Working effectively with university administrators," PhysTEC Annual Meeting, March 11-13, 2016, Baltimore (invited panelist).
44. "Tailoring properties of single and bilayer layer transition metal dichalcogenides: looking beyond graphene," U of Virginia Physics Colloquium, February 12, 2016.
45. "Easing pathway to physics teaching certification with a little help from PhysTEC," Winter 2016 Conference of the American Association of Physics Teachers, New Orleans, January 9-12, 2016.

2015

46. "Self-Learning Kinetic Monte Carlo method and its application to adatom-island diffusion and coarsening," CECAM/Psi-k Growth Simulation Workshop, Marburg, November 8-11, 2015.
47. "Tailoring properties of single layer MoS₂: looking beyond graphene," 3rd Euro-Mediterranean Conference on Materials for Renewable Energy (EMCMRE), Marrakesh, November 2-6, 2015.
48. "Self-Learning Kinetic Monte Carlo method and its application to adatom-island diffusion and coarsening," MRS Fall Meeting, Boston, Nov. 30 – Dec. 4, 2015.
49. "Tailoring characteristics of nanoparticles: size, shape, composition and environment matters," 250th ACS Meeting, Boston, August 16-20, 2015.
50. "Tailoring properties of single layer MoS₂: looking beyond graphene," Experimental Physics Seminar, University of Marburg, April 29, 2015
51. Reactivity of oxide and sulfide supported metal nanoparticles: role of the interface," From Witches Caldron to Material Science, Goslar, April 29-30, 2015.
52. "Ultrafast orbital charge dynamics and metallic domain growth in monoclinic VO₂," MURI Workshop of Ultrafast Science, University of Central Florida, November 12-13, 2015.
53. First International School on Computational Material Design," set of three invited talks, COMSATS Institute of Information Technology, Islamabad, Pakistan, May 25-29, 2015.
54. "Absorption Spectrum and Ultrafast Response of Monolayer and Bilayer Transition-Metal Dichalcogenides," Telluride Science Research Center Workshop on Nanomaterials: Computation, Theory, and Experiment, June 29 – July 4, 2015.
55. "Managing Faculty/Difficult Conversations," Physics Department Chairs Conference," American Physical Society, College Park, MD, June 5-7, 2015.

56. “Nano DMFT + DFTM: development of techniques beyond DFT,” DRC2015 Lake Arrowhead Conference on Materials Defect, June 7-12, 2015.

2014

57. “Tailoring properties of single layer MoS₂: looking beyond graphene,” Seminar, Department of Material Science, University of Texas, Austin, May 21, 2014
58. “Self-learning kinetic Monte Carlo simulations for heteroepitaxial systems: need lots of help from computer science thinking, IPAM Workshop, Lake Arrowhead, June 6-9, 2014.
59. “A Combined DFT+KMC Study of Selective Oxidation of NH₃ on rutile RuO₂(110) at Ambient Pressures,” DOE Contractors Meeting, Annapolis, July 20-23, 2014 (invited poster).
60. “Reactivity of oxide and sulfide supported metal nanoparticles: role of the interface,” 248th ACS Meeting, San Francisco, August 10-14, 2014.
61. “Single Layer MoS₂: Another Wundermaterial with Opportunities for Novel Electronic & Chemical Properties,” The Fourth Palestinian Conference on Modern Trends in Mathematics and Physics (PCMTMP-IV), Al-Quds University – Jerusalem, August 11-13, 2014 (via Skype).
62. “Tailoring properties of single layer MoS₂: looking beyond graphene,” International Materials Research Symposium, Cancun, August 18-21, 2014.
63. “Reactivity of oxide and sulfide supported metal nanoparticles: role of the interface,” CINVESTA, Merida, Mexico, August 22, 2014.
64. “Self Learning Kinetic Monte Carlo for epitaxial growth: can pattern recognition help us out?” Professor Vashishta Fest, USC, August 29, 2014.
65. “Exotic 2D Materials at the Frontiers of Nanoscience,” Science Café, UCF, September 18, 2014.
66. Should We Tell Our Daughters to Become Scientists? How can we change the climate in a Physics Department?, Seminar at Bochum, RESOLV Initiative, October 2, 2014.
67. “Tuning properties of single-layer transition metal dichalcogenides,” IUPAC NMS-X (Novel Materials Synthesis and Characterization Symposium), ZhengZhou, China, October 11-15, 2014.
68. “Adaptation of Dynamical Mean-Field Theory for Nanoscale Systems,” Computational Condensed Matter Physics Symposium, Tokyo, Japan, Dec. 2-4, 2014.
69. “Vibrational dynamics and thermodynamics as measures of nanoparticles structure,” 3rd International Workshop on Phonons, Krakow, Dec. 4-8, 2014.
70. “Challenges and Frontiers of Physics Research & Education,” COMSTECH Science Advisory Workshop, Islamabad, Pakistan, December 22-24, 2014.
71. “Tailoring properties of single layer MoS₂: looking beyond graphene,” Physics Colloquium, USC, Los Angeles, March 10, 2014.
72. “Manipulation of electronic and chemical properties of single layer MoS₂: insights from first principles calculations”, 247th American Chemical Society, Dallas, March 16-20, 2014.
73. “Tuning optical properties of arrays of pure and doped metallic nano chains,” 247th American Chemical Society, Dallas, March 16-20, 2014.

2013

74. “Manipulation of electronic and chemical properties of single layer MoS₂: insights from predictive modeling,” European-Mediterranean Conference on Materials for Renewable Energy, Istres, France, June 10-14, 2013.
75. “Manipulating electronic & chemical properties of single layer MoS₂,” Donostia International Center for Physics, San Sebastian, June 19, 2013.

76. "Electronic and chemical properties of single layer MoS₂: insights from ab initio electronic structure calculations, Marseille, June 25, 2013
77. "Band gap engineering in transition metal dichalcogenides," University of Genova, Italy, June 27, 2013.
78. "Computational design of functional nanomaterials: no longer a fiction," University of North Florida, Jacksonville, September 26, 2013.
79. Selectivity and reactivity of oxide-supported nanoparticles: role of the interface, Surface Chemistry Seminar, University of Liverpool, November 15, 2013.
80. "Role of Interface in the Methanol Oxidation for Oxide Supported Metal Nanoparticles", 246th American Chemical Society, Indianapolis, September 8 – 12, 2013 (presented by S. Hong).
81. "A Combined DFT+KMC Study of Selective Oxidation of NH₃ on rutile RuO₂ (110) at Ambient Pressures," 246th American Chemical Society, Indianapolis, September 8 – 12, 2013.
82. "Electronic and chemical properties of single layer MoS₂: insights from ab initio electronic structure calculations," IUPAC 9th Conference on Novel Materials (NMS-IX), Shanghai, October 17-22, 2013.
83. "Predictive modeling of materials for energy related needs," 60th Annual Meeting of American Vacuum Society, October 28 –November 1, 2013, Long Beach.
84. "The enticing features of oxides and sulfides: reactivity, selectivity and other matters," 245th Annual Fall Meeting American Chemical Society, New Orleans, April 7-11, 2013.
85. "Manipulating Electronic & Chemical Properties of Single Layer MoS₂," EMN Meeting, Orlando, April 9-12, 2013.
86. "Transforming a Physics Department," invited panelist at the Spring PhysTEC Meeting, Baltimore, March 15-17, 2013
87. "Single layer MoS₂: a promising material for nanoscience & nanotechnology," 2nd Symposium on Nanoscience and Nanotechnology, CNYN-UNAM, Ensenada, Baja California, March 4-8, 2013.
88. "Single layer MoS₂: insights from theory into another wunder-material," 53rd Sanibel Symposium, St. Simons Islands, GA, Feb 18-22, 2013.
89. "Computational design of functional nanomaterials: no longer a fiction," Southeastern Undergraduate Women in Physics Conference, Orlando, Jan 18-20, 2013.

2012

90. "Selectivity and reactivity of oxide surfaces: insights from *ab initio* calculations," Chemistry Colloquium, University of Pennsylvania, December 6, 2012.
91. The extended Self Learning Kinetic Monte Carlo Method: now lurking into 3D," Workshop on Defects in Materials, Institute for pure and Applied Mathematics, UCLA, October 25-30, 2012.
92. "Nanoscience and Nanotechnology: achievements & challenges," Plenary lecture, QAU-Tech, Workshop on Nanoscience and Nanotechnology, Quaid-e-Azam University, Islamabad, Pakistan, October 1-5, 2012.
93. "Computational Material Design," set of 3 invited talks, QAU-Tech, Workshop on Nanoscience and Nanotechnology, Quaid-e-Azam University, Islamabad, Pakistan, October 1-5, 2012.
94. Tuning optical properties of Au chains through transition metal atom doping," DOE Contractors Meeting, Theoretical Condensed Matter Physics, Rockville, August 19-22, 2012.
95. "Factors controlling some thermodynamic and chemical properties at the nanoscale: ab initio study of Pt and Pd nanoparticles," 244th Annual Fall Meeting American Chemical Society, Philadelphia, August 20 – 23, 2012
96. "Tuning optical properties of transition metal chains and their arrays," Third Palestinian Conference on Physics and Mathematics, Hebron, July 14 – 17, 2012.
97. Tuning optical properties of Au chains through transition metal atom doping," 16th International Conference on Thin Films and Solid Surface, Genova, July 1-6, 2012

98. "Tuning optical, magnetic and other interesting properties of nanoalloys for energy applications," NanoMexico12, Puebla, June 11-15, 2012.
99. "Optical properties of nanoalloys," Department of Physics, Aalto University, Espoo, Finland, January 16, 2012.
100. "Selectivity and Reactivity of oxide surfaces: insights from ab initio calculations," Colloquium Chemical Engineering Department, U of Florida, Gainesville, February 12, 2012.
101. Factors controlling the selectivity of oxide surfaces: results from DFT and KMC, 243rd ACS Annual Meeting, San Diego, March 25-30, 2012
102. "Tuning optical and other amazing properties of nanoalloy," Workshop on Nanoalloys, Brno, Czech Republic, April 2-4, 2012.

2011

103. "Density Functional Theory Method and its Applications," Workshop at National Center for Physics, Islamabad, Pakistan, December 28 – January 3, 2011 (set of 8 lectures).
104. "Selectivity and reactivity of oxide surfaces: insights from *ab initio* calculations," XVI Simposio en Ciencia de Materiales 2011,"Centro de Nanociencias y Nanotecnología – UNAM", Ensenada, Baja California, Mexico, 23-25 February 2011.
105. "Dynamical Mean-Field Theory for molecules and nanostructures," 51st Sanibel Symposium, Thematic Program on Magnetism and the Challenge of Nano-structures" 20-25 February, 2011.
106. (presented by postdoc Dr. Turkowski).
107. "Ab initio methods for examination of optical properties of nanomaterials for energy related application," 3 talks at 36th International Nathiagali Summer College, Pakistan, 1-5 July, 2011.
108. "Self-Learning Kinetic Monte Carlo Method and its application to adatom island diffusion and coarsening," ACCGE-18/OMVPE-15 Conference, Monterey, California, August 1-5, 2011.
109. "Nanoalloys: playing fields of Alchemists revisited and refined," Physics Colloquium, University of Missouri, Columbia, 12 September, 2011.
110. The Self Learning Kinetic Monte Carlo Method and its application to adatom island diffusion and coarsening on metal surfaces, Schloss Ringberg, October 16-19, 2011
111. "Engineering optical properties of nanomaterials for solar cell applications," US-Morocco Workshop on Nano-Materials & Renewable Energy, Al Akhawayn University, Ifrane, November 17 - 19, 2011
112. "Nanomaterials for solar cell applications," First Euro-Mediterranean Conference on Materials and Renewable Energies (EMCMRE-1), November 21-25, 2011

2010

113. "When gold is not gold anymore: size, shape and environment matters," Physics Colloquium, Florida Institute of Technology, February 20, 2010
114. "Selectivity and reactivity of oxide surfaces: insights from theory and modeling," Annual meeting of American Vacuum Society, Florida Chapter, March 8-10, 2010, Orlando.
115. "Nanoalloys: Playing fields of Alchemists revisited and refined," Physics Colloquium, University of Florida, April 1, 2010.
116. "Diffusion of large Molecules on Metal Surfaces: insights from ab initio calculations," Multiscale Modeling of Chemical Processes (MUMO), Turku, Finland, May 12, 2010.
117. "Adsorbates on metal surfaces: Much to learn from surface phonon dispersion curves even after all these years," D. L. Mills Symposium, University of California, Irvine, May 27-29, 2010.
118. "Diffusion of adatom clusters on metal surfaces: periphery diffusion or concerted motion?" International Conference on Modern Problems in Physics of Surfaces and nanostructures," June 8-10, 2010, Yaroslavl, Russia (presented by Dr. Trushin since I had to cancel the trip).

119. "Self learning Kinetic Monte Carlo technique: application to homo and hetroepitaxial growth on Cu and Ag surfaces," Telluride Workshop on Searching for Reaction Coordinates and Order Parameters, June 21-25, 2010, Telluride.
120. "Nanoscience for mankind," Salam Memorial lecture, Nathiagali, Pakistan, June 28, 2010.
121. Three lectures on Computational Material Design at 35th International Nathiagali Summer College, June 28 – July 3, 2010.
122. "Nanomaterials for mankind: fact or fiction," International Conference on Nano-Materials and Renewable Energies, Safi, Morocco, July 5-8, 2010.
123. "Atomistic Studies of Diffusion on Surfaces," 14th Workshop on Dynamical Phenomena on Surfaces, Schloss Ringberg, July 18-21, 2010.
124. "Self Learning Kinetic Monte Carlo Method and its application to cluster diffusion and island coarsening," 27th Max Born Symposium on Multiscale Modeling of Real Materials, Wroclaw, Poland, September 17-20, 2010.
125. "Nanoalloys: Playing fields of Alchemists revisited and refined," 2nd Palestinian Conference on Modern Trends in Mathematics and Physics, An-Najah National University, Nablus, Palestine, 2-4 August, 2010.
126. "Vibrational dynamics and diffusion of CO on metal surfaces: Ab initio atomistic simulation," 27th European Conference on Surface Science, Rotterdam, Netherlands, August 30 – September 3, 2010 (presented by postdoc M. Alcantara Ortigoza)
127. "Building functional material atom by atom: computational material design," XXX Meeting of the Mexican Society of Surfaces, September 27 -30, 2010, Playa Paraiso (plenary talk)
128. "Application of Density Functional Theory to examine surface reactivity," XXX Meeting of the Mexican Society of Surfaces, September 27 -30, 2010, Playa Paraiso (invited talk)

2009

129. "Nanoalloys: composition and local environment controlling properties," Bahauddin Zakia University, Multan, Jan 12, 2009.
130. "Science at the Nanoscale: Building the world atom by atom," Islamia University Bahawalpur, Jan 13, 2009
131. "Nanoscience and Nanopatterning", Discussion Leader, 2009 Chemical Reactions at Surfaces Gordon Research Conference, February 8 - 13, 2009, Ventura Beach.
132. "Nanoalloys: playing fields of Alchemists revisited and refined," Physics Colloquium, University of South Florida, February 20, 2009
133. "Diffusion of adatom clusters on metal surfaces: application of off lattice Self Learning KMC," Surface Kinetics International (SKI) Conference, March 20-22, 2009, Salt Lake City, Utah
134. "Nanoalloys: playing fields of Alchemists revisited and refined," Physics Colloquium, University of West Florida, April 6, 2009
135. "Policy and Chair Responsibilities," Leadership Excellence for Academic Diversity (LEAD) Workshop, Fayetteville, Arkansas, June 21-23, 2009
136. "Nanopatterning and its theoretical underpinnings," three lectures given at the 34th International Nathiagali Summer College, Pakistan, June 27 – July 4, 2009.
137. "Nanoalloys: playing fields of Alchemists revisited and refined," Seminar, Max Planck Institute fuer Festkorperforschung, Stuttgart, July 22, 2009
138. Invited Participant at DOE Workshop entitled "Discovery in Basic Energy Sciences: The role of computing at the extreme scale," August 12-15, 2009, Bethesda, MD.
139. "Challenges in academia for women of color" Fifteenth Annual faculty Diversity Institute on Teaching and Mentoring, October 23, Arlington, Virginia
140. "Ab-initio based kinetic Monte-Carlo simulation of Surface Phenomena," SFB Colloquium, Collaborative Research Center "Hierarchic Structure Formation and Function of Organic-Inorganic Nanosystems" (SFB 569), Ulm University, Germany, Dec 1, 2009.

141. "High CO tolerance of Pt/Ru nanocatalyst: Insight from first principles calculations," Workshop on Surface Science to Fuel cells: understanding microscopic processes, Regensberg Castle, Ulm, Germany, December 2-5, 2009
142. "High CO tolerance of Pt/Ru nanocatalyst: Insight from first principles calculations," Chalmers University, Goteborg, Sweden, Dec 14, 2009.

2008

143. "Senior Women in Physics: what the numbers tell us," "ADVANCE Workshop on Women in Science and Engineering, Kansas State University, February 16, 2008
144. "Factors controlling reactivity of surface oxides and other nanostructures," seminar, Dept. of Physics, Technical University of Denmark, Lyngby, Denmark, April 28, 2008
145. "Factors controlling reactivity of surface oxides and other nanostructures," seminar, Dept. of Physics, University of Aarhus, Denmark, April 30, 2008
146. "Some Ways in which Surface Oxides Facilitate or Hinder Reactions," seminar, Chemistry Department, Brook Haven National Laboratory, NY, March 26, 2008
147. "On Factors that may facilitate or hinder the Reactivity of Surface Oxides," Chemical Engineering Colloquium, University of South Florida, Tampa, April 20, 2008
148. "Electronic and geometric structure, dynamics, and thermodynamics of 34-atom Ag-Cu nanoalloy," 4th Annual Meeting of Florida Society for Materials Simulation, Tallahassee, May 5-7, 2008.
149. "Structure, dynamics, and vibrational entropy of bimetallic nanoalloys," seminar, Institut für Festkörper Physik, Forschungszentrum-Karlsruhe, Germany, June 16, 2008.
150. Three lectures on "Computational methods for nanoscale material design," 33rd International Nathiagali Summer College, Pakistan, June 28 – July 5, 2008.
151. "Microscopic processes responsible for the diffusion of Cu/Ag adatom islands on Ag(111)/Cu(111): insights from theory," Nanoscale Spectroscopy and Nanotechnology (NSS5), Athens, Ohio, July 15-19, 2008.
152. "Nanoalloys: playing fields of our fore-fathers "the Alchemists" revisited and refined," Physics Colloquium, University of Delaware, October 3, 2008
153. "Women of Color in Academia: way forward," 15th Institute on Teaching and Mentoring, Southern Regional Education Board, Tampa, Florida, October 26, 2008.
154. "Self Learning Kinetic Monte Carlo Simulations: application to hetero- and homo-epitaxial growth processes," 4th International Conference on Multiscale Modeling of Materials, Tallahassee, October 27-31, 2008.
155. "Nanoalloys: playing fields of Alchemists revisited and refined," Physics Colloquium, Temple University, Philadelphia, December 1, 2008.

2007

156. "Fuel Cells: a theoretical perspective," 32nd International Nathiagali Summer College, Nathiagali, Pakistan, June 25-30, 2007.
157. "Fuel Cell Reactions: some basics of theoretical calculations," 32nd International Nathiagali Summer College, Nathiagali, Pakistan, June 25-30, 2007.
158. "Theoretical Understanding of Reactions in Fuel Cells," 32nd International Nathiagali Summer College, Nathiagali, Pakistan, June 25-30, 2007
159. "Factors controlling the rates of chemical reactions on nanostructured surfaces: insights from theory," 7th International Workshop on Surface Physics, Polanica Zdroj, Poland, September 5-9, 2007.
160. "Self Learning Kinetic Monte Carlo Simulations and its Application to Epitaxial Growth Processes," ICIAM (International Council for Industrial and Applied Mathematics) 2007 Symposium, Zurich, July 15-20, 2007.

161. "Electronic and Geometric Structure, and Thermodynamics of Ag-Cu Nanoalloys," Condensed Matter Physics Seminar, Catholic University, Santiago de Chile, December 4, 2007.
162. "What can we still learn from the dispersion of surface phonons?" (with Sampyo Hong), 12th International Conference on Vibrations at Surfaces, Erice, Italy, July 21-26, 2007.
163. "Novel Properties of Alloy Nanoparticles," Inaugural Symposium, National Center for Physics, Islamabad, Pakistan, March 26-29, 2007.
164. "Self Learning Kinetic Monte Carlo Simulation and its Application to Cu Cluster Diffusion on Cu(111)," Florida Society of Materials Simulators (FSMS) 2007, Annual Meeting, Tampa, Florida, June 6-8, 2007.

2006

165. Sigma Xi Distinguished lecture, University of Maine, March 2006, "Science at the nanoscale: promising facts or fiction?"
166. "Computational material design: challenges and prospects," Physics Colloquium, University of Central Florida, April 1, 2006.
167. "Science at the Nanoscale: Building Functional Materials Atom by Atom," Laboratory for Surface Modification and Sigma Xi Distinguished Lecture, Rutgers University, Feb 15-16, 2006
168. Sigma Xi Distinguished Lecture "Science at the Nanoscale: Promising Facts or Fiction?" University of Colorado, April 17, 2006.
169. "Science at the Nanoscale: Building Functional Materials Atom by Atom," Physics Colloquium, University of New Mexico, April, 2006
170. "Periphery motion or collective diffusion: the case of adatom islands on metal surfaces," 232nd ACS Annual Meeting, San Francisco, November 2006
171. "Anharmonic effects at metal surfaces," Workshop on Surface Dynamics, Modena, July 2006.
172. "Diffusion of two-dimensional adatom clusters on metal surfaces: application of the Self Learning Kinetic Monte Carlo method," International Conference on Solid Films and Surfaces, Prague, July 2006
173. "Molecular dynamics simulation of surface melting and roughing transitions," Workshop on Computational Material Science, JNCASR, Bangalore, July 6-10, 2006
174. Three lectures on computational nanoscience at the International Nathiagali Summer College, July 2006.
175. "Tracking the motion of adatom clusters on fcc(111) surfaces: results from on-lattice and off-lattice SLKMC," CMSN-2006 workshop, University of Maryland, October 6-7, 2006.
176. "Theoretical and Computational Studies of the Initial Stages of Thin Film Growth," CIIT-ISESCO International School on Surfaces, Thin films, Nanostructures and their applications, Lahore, Pakistan, Oct. 27-Nov. 1, 2006.

2005

177. 3rd US – Africa MRS Meeting and Workshop on Nanoscience and Nanotechnology, Dec 6-10, 2005, Marrakesh, "Computational Nanoscience: designing materials atom by atom."
178. 55th Midwest Solid State Conference, October 8-9, Columbia, Missouri, "Cluster Diffusion and Coalescence on Metal Surfaces using a Self Learning Kinetic Monte Carlo Method."
179. Sigma Xi Distinguished lecture, University of Vermont, September 22, 2005, "Should we tell our daughters to become scientist?"
180. Sigma Xi Distinguished lecture, Norwich University, Vermont, September 21, 2005, "Science at the nanoscale: promising facts or fiction?"
181. International Workshop on Surface Physics (Advanced and Bio-Materials), Polanica Zdrój, Poland, 10-13 September 2005, "Atomistic studies of adatom- and vacancy-cluster diffusion and coalescence on Cu(111) using a self-learning kinetic Monte-Carlo method."

182. Solid State Physics Seminar, University of Twente, Netherland, July 20, 2005, "Atomistic studies of cluster diffusion and coalescence on metal surfaces."
183. 30th International Nathiagali Summer College, Nathiagali, Pakistan, July 3-9, 2005, set of four lectures on "Theory and modeling of materials at the nanoscale."
184. Sigma Xi Distinguished lecture, University of Wisconsin-Fox Valley, May 9, 2005, "Should we tell our daughters to become scientist?"
185. Sigma Xi Distinguished lecture, University of Wisconsin-Oshkosh, May 8, 2005, "When gold is no longer gold: a peek at matters at the nanoscale."
186. Speaker at a Symposium on "Women Scientists on Gender, Race, and Nationality," Massachusetts Institute of Technology, Boston, April 29-30, 2005.
187. Sigma Xi Distinguished lecture, Texas Christian University, April 22, 2005, "Science at the Nanoscale: promising facts or fiction?"
188. Sigma Xi Annual Distinguished lecture, University of Puerto Rico, Mayaguez, April 21, 2005, "When gold is no longer gold: on tailoring properties of materials",
189. Sigma Xi Distinguished lecture, Emporia State University, Emporia, Kansas, April 16, 2005, "Science at the nanoscale: promising facts or fiction?"
190. Sigma Xi Distinguished lecture, Miami University, March 8, 2005, "Science at the nanoscale: promising facts or fiction?"
191. Sigma Xi Distinguished lecture, Corning Chapter, March 4, 2005, "Should we tell our daughters to become scientist?"
192. Colloquium, Corning Glass Industry, March 3, 2005, "Science at the Nanoscale: site selective properties controlling reactivity, morphology, and growth patterns on nanostructures."

2004

193. Annual Meeting of Materials Research Society, Boston, Nov 29 – Dec. 2, 2004, "Cluster Diffusion and Coalescence on Metal Surfaces: Applications of a Self-Learning Kinetic Monte-Carlo Method."
194. Sigma Xi Annual Distinguished Lecture, University of Kansas Medical Center, November 16, 2004, "Can nanotechnology keep us healthier?"
195. CECAM Workshop on In situ atomic scale characterization of surfaces under high pressures: recent advances in experiment and theory, Lyon, November 4-6 2004, "A comparative ab initio study of the reactivity of CO and NO on RuO₂ (110)."
196. Sigma Xi Distinguished Lecture, University of Missouri-Columbia, October 28, 2004, "Promises of Physics at the Nanoscale: fact or fiction?"
197. Sigma Xi Distinguished Lecture, Army Research Laboratory, Maryland, September 30, 2004, "Promises of Physics at the Nanoscale: fact or fiction?"
198. Workshop on Nanomagnetism and the Advanced Photon Source at Argonne National Laboratory, Lake Geneva, Wisconsin, Aug. 29- Sept 1, 2004, "Single Molecule Magnets: some prospects, some challenges."
199. Annual Meeting of SPIE (Society of Optical Engineers), August 2-6, 2004, Denver, "Atomistic Modeling of Thin Film Growth Modes"
200. CMNRS Seminar, Marseille, July 19, 2004, "Site Selectivity in Chemical Reactions on Stepped Metal Surfaces."
201. Electrical Engineering Department Seminar, Lappeenranta University of Technology, Finland, June 29, 2004, "On theoretical measures of the reactivity of metal surfaces."
202. Fysik Laboratory Seminar, Helsinki University of Technology, June 28, 2004, "Diffusion of Two dimensional Cu Clusters on Cu(111)."
203. Chemical Physics seminar, Fritz Haber Institute, MPG, Berlin, July 21, 2004, "On poisons and promoters: theoretical measures of reactivity of metal surfaces."

204. Annual Meeting of the European Material Research Society (E-MRS), May 25-28, 2004, Strasbourg, "Cluster Diffusion and Step Fluctuations on Metal Surfaces: applications of a Self-learning Kinetic Monte-Carlo method."
205. Workshop on Nanoscience and Nanotechnology, Islamabad, Pakistan, April 11-16, 2004, "Physics at the nanoscale: set of 3 lectures."
206. Collective Aspects of Stochastic Non-equilibrium Phenomena at Surfaces and Interfaces, Lorentz Center, Leiden University, 14-25 June 2004, "Adventures in Surface Diffusion with a Self-Learning Kinetic Monte Carlo Technique."
207. 17th Workshop in Recent Developments in Computer Simulational Studies, University of Georgia, Athens, Feb. 16-20, 2004, "Towards a self teaching approach to the kinetic Monte Carlo method"
208. Physics Colloquium, Washington University, St. Louis, March 4, 2004, "Physics at the nanoscale: where is the beef?"

2003

209. American Chemical Society, Annual Meeting, New Orleans, March 23-27, 2003, "On surfaces and nanostructures: under-coordination controlling the chemistry."
210. International Workshop on Surface Physics, Worslaw, Poland, September 12-15, 2003, "Site selectivity in chemisorption on metal surfaces: on poisons and promoters."
211. International Workshop on Fundamental Aspects of Surface Diffusion, Trest, Czech Republic, Sept. 14-17, 2003, "Insights from the diffusion of two dimensional Cu clusters on Cu(111)."
212. University of Toledo, Physics Colloquium, November 20, 2003, "Physics at the Nanoscale: promising fact or fiction?"
213. Workshop on Fundamental Issues in Nonequilibrium Interface Dynamics, University of Maryland, October 20-24, 2003, "Towards a Realistic Approach in Atomistic Studies of Diffusion and Fluctuations on Metal Surfaces."
214. Department of Applied Physics, Chalmers University of Technology, Goteborg, Sweden, May 22, 2003, "Role of undercoordination in determining the chemical reactivity of vicinal surfaces."
215. Laboratory of Physics Seminar, Helsinki University of Technology, June 16, 2003, "Optical Recognition of Steps on Metal Surfaces."
216. Department of Physics, Oulu University, Oulu, Finland, June 19, 2003, "On Poisons and Promoters on Stepped Pd Surfaces."
217. Second International Conference on Physics Education in Developing Countries, Karachi, Pakistan, February 7-10, 2003 "Concepts in physics: some simple class room demonstrations that get the point across."
218. 28th International Nathiagali Summer College, Pakistan, June 24 – July 1, 2003 "Computational Techniques in Nanoscience and their Applications."

2002

219. Department of Chemistry, University of California, Riverside, December, 2002, "Role of under-coordinated sites in chemisorption and surface stability."
220. Department of Physics, University of Kansas, Lawrence, December, 2002, "Are we sacrificing science by jumping on the nano-bandwagon?"
221. Department of Physics, University of Rochester, Rochester, November, 2002, "Physics at the nanoscale: promising fact or fiction?"
222. Fritz Haber Institut, Berlin, July, 2002, "Does the corner kick control the game or is it the local coordination?"
223. Karachi University Colloquium, January, 2002, "Challenges and opportunities in physics education."
224. 27th International Nathiagali Summer College

2001

225. Department of Physics, Technical University of Denmark, January 19, 2001, "Vibrational Dynamics and Thermodynamics of Surfaces and Nanostructures".
226. NSF's Workshop on Partners in Nanotechnology, January 28-29, 2001, "Evolution of Nanoscale Film Morphology."
227. Ioffe Institute for Physics, Leningrad, Russia, April 17, 2001, "Finite Temperature Studies of Surfaces and Nanostructures".
228. Institute for Microelectronics, Yaroslavl, Russia, April 19, 2001, "Atomistic Studies of Epitaxial Growth on Metal Surfaces".
229. Department of Physics, Chalmers University, Goteborg, Sweden, May 11, 2001, "Self diffusion of Adatoms and Vacancies of Metal Surfaces: Paths, Processes and Diffusion Prefactors"
230. Physik Institut der Universitaet Zuerich, May 17, 2001, "Vibrational Dynamics and Thermodynamics of Surfaces and Nanostructures".
231. Series of 4 lectures on "Theoretical Methods for Calculating Finite Temperature Properties of Surfaces and Nanostructures", Fritz Haber Insitute, Berlin, May, 2001.
232. Annual Meeting of Alexander von Humboldt Foundation, June 2001, Berlin, "AvH Fellowship, AvH Forschungspreis, where do we go from here?"
233. Tenth Workshop on Dynamics at Surfaces, El Escorial, Spain, June 13-16, "Anharmonic Effects at Surfaces: temperature dependence of surface phonon linewidths."
234. 26th International Nathiagali Summer School, Nathiagali, Pakistan, June 26-July 5, 2001;
235. four lectures on "Microscopic Processes Responsible for Thin Film Growth."
236. Workshop on Characteristics of Stepped Cu Surfaces, University of Erlangen-Nuernberg, July 22-23, "Dynamics and Thermodynamics of Stepped Cu Surfaces".
237. Physik Department T30, Technische Universitaet Muenchen, July 24, 2001, "Novel properties of nanostructures: results of microscopic studies".

2000

238. NATO Advanced Research Workshop on Collective Diffusion and Nonequilibrium Phenomena at Surfaces, Prague, Czech Republic, October 2-6, 2000; "Paths, barriers and pre-exponential factors for self-diffusion on metal surfaces."
239. Seventh International Summer School, "Nicolas Cabrera" on "Imaging and Manipulation of Matter at the Nanometer Scale," Madrid, Spain, September 11-15, 2000: "Tip Induced Manipulation of Atoms on Surfaces."
240. 25th International Nathiagali Summer School, Nathiagali, Pakistan, June 26-July 5, 2000; three lectures on Nanotribology.
241. Laboratory of Physics Seminar, Helsinki University of Technology, September 19, 2000, "Thermodynamics of Nanocrystals."