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 (now Quaid-e-Azam University), Islamabad
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

2021 - Trustee Chair Professor, University of Central Florida
2012 - Pegasus Professor, Department of Physics, University of Central Florida
2015 - Lead, 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

Visiting Professor, Carl von Ossietzky Universität Oldenburg, July-August 2022, April-June 2024
Miller Visiting Professor, University of California Berkeley, Spring Semester, 2018
Visiting Scientist, Aalto University, Espoo, Finland, March-June 2017; December 2017; June 2018
Visiting Scientist, Donostia International Physics Center, San Sebastian, Dec. 2016 – present
Visiting Scientist, Max Planck Institut für Festkörperforschung, Stuttgart, July, July 2019
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

2023 Chair, Division of Computational Physics (DCOMP) American Physical Society
2022 Research Incentive Award, University of Central Florida
2022 Mentor of the Year, American Vacuum Society

2022 Helene Lange Visiting Professorship, Carl von Ossietzky Universität Oldenburg
2021 Fellow, American Association for the Advancement of Science (AAAS)
2021 Vice Chair, Division of Computational Physics (DCOMP) American Physical Society
2020 Senior Mercator Fellow, Ruhr University-Bochum, Germany
2019 Fellow, Royal Society of Chemistry (UK)
2018 Miller Visiting Professor, University of California, Berkeley
2018 APS Apker Award Committee (3 years)
2018 Chair, Diversity & Inclusion Committee, American Vacuum Society (3 years)
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 Physical Sciences Advisory Board Member, Oak Ridge National Laboratory (ongoing)
2017 Founding Section Editor, Journal of Physics Condensed Matter: physics of chemical processes
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
2009 Editorial Executive Board Member, Journal of Physics Condensed Matter, IOP, UK (ongoing)
2007 Sigma Pi Sigma Member, Honorary Member, UCF
2003 Phi Beta Kappa, Honorary Member, Beta Chapter
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 Commerce Bank Distinguished Graduate Faculty Award, Kansas State University
1998 Fellow, American Physical Society
1993 CNRS-Italy Fellowship for collaborative research
1987 Alexander von Humboldt Research Fellowship, Germany, 1987-88

SELECTED AWARDS THAT INVOLVE LECTURING

2022 Helene Lange Visiting Professorship, Carl von Ossietzky Universität Oldenburg
2020 Senior Mercator Fellow, Ruhr University-Bochum, Germany
2004 Sigma-Xi Distinguished Lecturer (2004-2006)
1997 Presidential lecturer, Kansas State University (continued till 2006)
1994 UNDP-TOKTEN Fellowship, Quaid-e-Azam University, Islamabad, Pakistan
1992 Stamey Undergraduate Teaching Award, Kansas State University
1998 - 2012 Lecturer, International Nathiagali Summer College, Pakistan (delivered 3-5 lecturer per year)

SCIENTIFIC PRODUCTIVITY

Publications: total over 320 in refereed high impact journals.
Citations from Google Scholar: 12591; *h-index*: 60
https://scholar.google.com/citations?user=ted1v6oAAAAJ&hl=en
Invited Presentations: on average about 12 – 20 invited talks per year.

PRINCIPAL RESEARCH TOPICS

Predictive modeling of 2-dimensional materials, with/without defects, for optoelectronics & catalysis
Multi-scale modeling of chemical reactions and related phenomena at surfaces
Development of techniques beyond density functional theory for strongly correlated materials
Development of techniques for non-equilibrium phenomena, quantum excitations & excited states
Rational designing of hybrid interfaces: molecular magnetic structures – semiconductors/metals
Theory and modeling of single atom catalysts (supported on oxide surfaces)
Understanding processes that control growth and morphological evolution of nanostructures
Surface coordination chemistry: novel functionality via substrate charge transfer and oxidation state
Understanding and predicting the response of surfaces and nanostructures to ultrafast external fields
Ab initio modeling of electrochemical reactions and the chemical environment

CURRENT & RECENTLY FUNDED PROJECTS (2017 – present)

- DOE: DE-SC0024083 "*Theoretical and experimental investigations of the electrocatalytic environment for sustainable fuel production,*" (9/1/2024 – 8/31/27): PI
- DOE: DE-FG02-07ER46354 "*Theoretical and Computational Studies of Excitations and Excited States in Functional Nanomaterials*" (1993 - present): PI
- NSF: CHE-2400068 "Understanding and Predicting Reactivity and Selectivity of Supported Few Atom Catalysts through Control of their Local Environment" (9/1/24 - 8/31/27): PI
- DOE-EFRC "*Center for Molecular Magnetic Quantum Materials*" located at University of Florida, (9/1/2018 – 8/31/2024): Co-PI with 10 other Co-PIs; PI: Cheng (UF)
- NSF: CHE-1955343 *"Understanding and Predicting Reactivity and Selectivity of Single Atom Catalyst,"* (9/1/2020-12/31/2024): PI; Co-PIs Liu (UCF), Hong (Brewton Parker College)
- NSF: DMR-1710306 "*Collaborative Research- Connecting Mesoscale Dynamics of Metallic Films on Semiconductors to Nanoscale Phenomena*," (9/1/2017 – 12/31/2021) with Chiang & Fong (UC Davis)
- DOE: DE-FG02-07ER15842 "*Controlling Structural, Electronic, and Energy Flow Dynamics of Catalytic Processes through Tailored Nanostructures*" (9/15/2003 – 9/14/2020): PI; Co-PIs: Bartels (UC Riverside), Blair (UCF) & Dowben (U Nebraska); previous Co-PIs Heinz (Columbia) and Chen (U South Carolina)
- NSF: CHE-1465105 "*SusChEM Defect-laden 2D Catalysts for Carbon Sequestration and Safer Hydrogenation*" (8/1/2015-7/31/2020) Co-PI; PI: Blair (UCF), Co-PI: Tetard (UCF)
- NSF: DUE-1246024 "*Active Learning Strategies for Algebra-based Introductory Physics Courses at UCF*" (7/1/2013-6/30/2017) PI; (Co-PIs: Chini, Kara, Flitsiyan, Dubey)
- APS Site Grant: "UCF PhysTEC Comprehensive Site," (7/1/2013-); first three years funded by APS and UCF; continues to be funded by UCF (with support of UCF PhysTEC team).
- APS Site Grant: "UCF APS-Bridge Program Site" (7/1/2015-); first three years funded by APS and UCF; continues to be funded by UCF (with support of UCF Physics Bridge team).

EXTERNAL RESEARCH FUNDING credited to Talat Rahman at UCF (2007-present): **over $ 12.5 M**

GRADUATE STUDENTS SUPERVISED

Jin He, Ph.D., 1987
Liqui Yang, Ph.D., 1991
Kai Yang, Ph.D., 1991
Wes Bailey, MS, 1995
Neha Nayyar, PhD, 2014
Alamgir Kabir, PhD, 2015
Ghazal Shafai, PhD, 2016
Jarrad Pond, PhD 2016

Pavlin Staikov, Ph.D., 1998
Sondan Durukanolgu, Ph.D., 1999
Ahlam Al-Rawi, Ph.D., 2000
Weibin Fei, Ph.D., 2000
Chandana Ghosh, PhD, 2003
Sampyo Hong, PhD, 2005
Faisal Mehmood, PhD, 2006
Altaf Karim, PhD, 2006
Marisol Alcantar Ortegoza, PhD, 2007
Handan Yildirim, PhD, 2010
Duy Tran The Le, PhD, 2012
Maral Aminpour, PhD, 2013
Syed Islamuddin Shah, PhD, 2013
Mario. Hernandez, visiting student 2013-2015
S. Faiza Sherazi, PhD in progress
Takat Rawal, PhD 2017
Shree-Ram Acharya, PhD 2018
Zahra Hooshmand, PhD 2018
Tao Jiang, PhD 2019
Nasim Uddin, PhD 2020
Mahboob ur Rehman, PhD 2021
Andre Childs, MS 2018
Rainier Berkley, MS 2018
Dave Austin, PhD 2024
Eric Switzer, PhD 2023
Theodoros Panagiotakopoulos, PhD in progress
Jia Shi, visiting student 2019 - 2022
Bushra Ashraf, PhD in progress
John Janish, PhD in progress
Adolfo Partida, PhD in progress

POST-DOCTORAL ADVISEES AND SENIOR RESEACH ASSOCIATES

Dr. Sergey Stolbov, 2000 - 2007
Dr. Zengju Tian, 1993
Dr. Abdelkader Kara, 1994 – 2007
Dr. Ulrike Kürpick, 1995-98
Dr. Ahlam Al-Rawi, 2003- 2009
Dr. Vasse Chis, 2009 – 2010
Dr. Chandana Ghosh, 2008-2011
Dr. Alfredo Ramirez, 2012-2014
Dr. Mario. Hernandez, 2019-2020
Dr. Joseba Alberdi, 2017 – 18
Dr. Jia Shi, 2022 – 2023
Dr. Dave Ausin, 2024 - 2025
Dr. Duy Le, 2012 – (Assistant Scientist)
Dr. Volodymyr Turkowski, 2008 – (Assis Research Prof.)
Dr. Marisol Alcantara Ortigoza, 2008 – 2012
Dr. Giridhar Nandipati, 2009 – 2012
Dr. Sampyo Hong, 2005 – 2014
Dr. Jacquelyn Chini, 2010 - 2012
Dr. Zahra Hooshmand, 2019 - 2020
Dr. Shree-Ram Acharya, 2018 – 2019
Dr. Tao Jiang, 2020 - 2021
Dr. Tyler Campbell, 2021 - 2022
Dr. Eric Switzer, 2023 - 2024

UNIVERSITY SERVICE

***At the University of Central Florida*:**

Search Committee Chair, REACT Cluster Faculty Position, 2025
Search Committee Member, Theoretical Catalysis Science Faculty Position, 2025
Chair, COS Adhoc Space Evaluation Committee, 2025
Chief Negotiator, UFF-UCF, 2020 - 2024
Faculty Compliance Advisory Committee, 2017 – 2019
Lead for UCF Faculty Cluster on Renewable Energy and Chemical Transformations (REACT), 2017 –
Search Committee Chair for 5 REACT Faculty Positions, 2017 - 2019
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 and 2019
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

***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 Biochemist, 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):

- Chair Line, Division of Computational Physics, American Physical Society, 2021 - 2025
- Chair, Diversity and Inclusion Sub Committee, American Vacuum Society, 2018 – 2021
- Member, Multi Society Diversity Council, USA, 2018 - 2024
- 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.
- Physics Graduate Program Reviewer, Clemson University, 2021-2022
- Reviewer for Nebraska Center for Energy Sciences Research, January 20-22, 2021
- External advisor for the establishment of Material Science and Engineering PhD Program, University of Massachusetts, Amherst, October 2021
- 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.

For the US Department of Energy and National Science Foundation:

- Regular reviewer on DOE-BES panel reviews. Recent panels include:
    - NSF Science & Technology Center, University of Michigan, May 5-6, 2025
    - NSF MRSEC, Ohio State University, May 2024
    - INCITE Condensed Matter Physics Program, 2021 -2024 (panel Member)
    - INCITE Material Science initiative, 2011, 2012 (panel Chair)
    - INCITE Material Science initiative, 2009, 2010 (panel Member)

    - SUNCAT Research Center, Stanford University/SLAC, April 2016.
    - BES Division, Energy Frontier Research Centers mid-term review, February 2016.
    - 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.
- Served as reviewer for several recent high-profile initiatives:
    - DOE Quantum Information Science (QIS) FOA, 2021
    - DOE Catalysis Science Early Career Proposals, 2017- present
    - DOE Earth & Geo Science Early Career Proposals, 2020
    - DOE Polymer Upcycling FOA, 2021
    - DOE Chemical & Biological Sciences Early Career Proposals, 2019 -
    - DOE Computational Materials Sciences Centers, 2017 -
    - NSF Science & Technology Center Proposals, 2019
    - NSF Center for Chemical Innovation (CCI), 2019
    - NSF DMREF program, 2017
    - DOE Office of Science Graduate Fellowship Program (DOE SCGF)
    - DOE ASCR Leadership Computing Challenge (ALCC) program
    - DOE Computational Chemical Sciences FOA
    - NSF Early Career Proposals in several Divisions, regularly for the past 20 years

- Invited participant, NSF Metals and Metallic Nanostructures Workshop, July 19-22, 2021
- 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; invited also in 2019 (had to decline because of COI).
- 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
- Frequent reviewer of research proposals from many federal agencies
- Ongoing evaluation panel member for NSF funding initiatives such as NIRT, IGERT, MRI, CDI, MRSEC, DMREF, STC, CCI

For American Physical Society:

- Chair, APS Fellow Selection Committee for DCOMP, 2024-25
- Program Committee (DCOMP) APS Global Summit March 2025
- APS Site visit team
- Vice Chair/Chair-Elect/Chair/Past Chair, Division of Computational Physics 2021 - 2025
- Vice Chair / Chair, Davisson and Germer Prize Committee, 2015-2017
- Vice Chair/Chair-Elect/Chair Topical Group on Energy Research and Applications 2014-2016
- Member, APS Aneesur Rahman Prize Committee, 2021
- Member, Apker Research Award Committee, 2018 – 2021
- Program Chair (DCOMP) APS March Meeting, 2023 & 2024
- Helped organize the First Annual IGEN Meeting, Orlando, Florida, October 25-27, 2019
- Helped organize Annual National Mentoring Conference, Orlando, Florida, February 6-8, 2020
- 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.
- Organized GERA Symposium on "Materials for Sustainable Development," APS March Meeting 2016, Baltimore.
- Organized GERA Symposium on "Energy: Renewable and Sustainable," APS March Meeting 2017, New Orleans.

For American Vacuum Society:

- Chair, Diversity and Inclusion Sub Committee 2018 – 2021 (facilitated its conversion to a standing committee; initiated efforts to enhance diversity & inclusion at annual meetings)
- Member, Diversity, Equity and Inclusion Committee, AVS, 2021 -
- Member, National Multi-society Diversity Committee, 2018 –
- Organized Round Table Discussion on "Diversity & Inclusion: some best & worst practices," 65th AVS International Symposium &Exhibit, Long Beach, October (2018).
- Organized Round Table Discussion on "Diversity & Inclusion: some best & worst practices," 66th AVS International Symposium &Exhibit, Columbus, Ohio, October (2019).
- 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

- RED19, Review Panel for Physics and Mathematics Departments, University of Gothenburg, Sweden, 2019-20.
- One of three international experts invited to advise Physics Department Faculty Hiring Committee, Tampere University, Finland, on tenure-track faculty candidates, April 2018.
- Reviewed proposals for Luxemburg Science Foundation and Swiss Science Foundation, 2020
- Reviewed proposals for Polish Science Foundation and European Research Council, 2021
- One of three international experts invited to advise University of Gothenburg, Sweden, on the establishment of a Marine Sciences Department, October 2014.
- Chair, RED10, 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 - .
- "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. Sikandar Hayat, Bahawalpur University, Pakistan, 2012
    c. Dr. Zakir Hussain, Bahawalpur University, Pakistan, 2016
    d. Dr. Waqas Hussain, COMSATS Institute of Technology, 2012.
    e. Dr. Samia Ahmed, COMSATS Institute of Technology, 2019.
    f. Dr. Aldo Ugolotti, University of Milano-Bicocca, 2019

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

- Regular organizer of scientific and educational workshops and forums in Islamabad and Karachi, Pakistan (2-3 a year).
- Member, International Organizing Committee, International Conference on Solid Films and Surfaces 2012-present.
- Organizer, 79th Physical Electronics Conference, Orlando, Florida, June 2-6, 2019.
- 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):

- As site leader of the APS Bridge Program grant (3 years APS + UCF long term commitment), 2015 to present, engaged in establishing policies and procedures that help recruit and retain physics graduate students from underrepresented minority (URM) groups. A total of 49 URM students have been admitted to the Physics Department at UCF since 2014. At least 2 to be admitted per year for the next five years. Three have already graduated with PhD. The percentage of URM students in the UCF Physics Department has increased from ~3% in 2014 to 22% in 2020.
- Invited to Virginia Tech University, May 3-5, 2016, to advise faculty and administrators on strategies that help recruit and retain URM students.
- Helped establish in 2012 the Women in Physics Society (WPS) 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 WPS, facilitated the organization of the 2013 South-eastern Conference for Undergraduate Women in Physics at UCF. About 120 women engaged in an exciting workshop with 18 successful female physicists.

- 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 an 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 PI of the APS PhysTEC Comprehensive Site grant, 2013 – present, engaged in recruitment and training of physics majors who might be interested in careers in teaching to address the national issue of shortage of teachers with sound content knowledge. In this regard, the UCF Physics Teacher-in-Residence program has strengthened interactions with local high school teachers, leading to additional mentoring and training of interested students. UCF Physics Department is now one of the few in the country that produces 5 or more physics majors per year who adopt physics teaching as career.
- Helped establish and sustain (2011 – present) 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.

- Led NSF-supported pedagogy reform in introductory physics courses via implementing an active learning environment (studio) and inquiry-based methodology. Also facilitated instructional reforms in upper-division physics courses.

SOME HIGHLIGHTS of ADMINISTRATIVE AND LEADERSHIP EXPERIENCE

- As chair of Physics Department, University of Central Florida (2006 – 2015) helped:
    - triple the number of PhD students (with increasing gender balance)
    - triple the number of physics majors
    - increase departmental external funding 8-fold (in 5 years)
    - establish APS-UCF funded Bridge Program for recruiting URM graduate students
    - establish APS-UCF funded PhysTEC Program for physics majors for careers in education
    - establish vibrant research groups in Ultrafast Science and Physics Education
    - interdisciplinary research programs with other departments
    - transform introductory physics pedagogy into one with emphasis on active learning
- Led UCF wide effort to establish a Research Cluster in Catalysis for Energy (5 new faculty hired)
- As president (elect/present/past) of Faculty Senate at Kansas State University (1997-2000) led
    - an equity study that helped resolve some long-standing issues
    - a productive solicitation with the Athletics Department for university library funding
    - a successful effort to reform faculty Tenure and Promotion Regulations
    - a fruitful negotiation with university administration on Faculty Grievance Procedures

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)
- Royal Society of Chemistry, UK
- PhysTEC (Physics Teachers Education Coalition): aimed at increasing number of physics teachers by recruiting and training physics majors for careers in teaching)
- APS Bridge Program (aimed at increasing number of physics PhDs from underrepresented minority groups)
- National Mentoring Community established 2015 by American Physical Society
- Multi Society Diversity and Inclusion Committee
- AIP Liaison Committee on Underrepresented Minorities (LUCURM)

LANGUAGES SPOKEN

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

INVITED TALKS (2000 – present)

1. Understanding the electrochemical environment for CO2RR & HER, PCTC 25 Conference, University of Pennsylvania, May 3-4, 2025
2. Novel 2D Materials for a Sustainable Future, Physics Colloquium, Indiana University Indianapolis, April 24, 2025
3. A walk through the world of reduced dimensionality in search of materials with novel functionality, Physics Colloquium, Rensselaer Polytechnic Institute, April 9, 2025

2024

4. Novel Low Dimensional Materials for a Sustainable Future, Bose Centennial Celebration –the legacy, Dhaka University, November 7 - 10, 2024
5. Designing the local environment of single atom catalysts for product selectivity: theory meets experiment, AVS 70 Symposium & Exhibition, Tampa, November 3-8, 2024
6. Tuning the local environment of single atom catalysts for enhanced reactivity and selectivity, Physics Seminar, University of Genoa, September 10, 2024
7. Enhanced reactivity of oxide-supported bimetallic and single atom sites: insights from the local atomic environment, IMN 2024, Genoa, Italy, September 4, 2024
8. Excited state charge dynamics in 2D materials: interplay of excitons & phonons, Priya Vashishta 80th Birthday Research Symposium, USC, August 9, 2024
9. Excited state charge dynamics and optical response in 2D materials: interplay of excitons & phonons, Max Planck Institute for Research in Solid State Physics, Stuttgart, July 23, 2024
10. Spin crossover molecules for low power nonvolatile memory, Physical Chemistry 1 Seminar, Ruhr University Bochum, July 31, 2024
11. Excited state charge dynamics and optical response in 2D materials: interplay of excitons & phonons, Physik Seminar Phillipps Universität Marburg, July 22, 2024
12. Science for Society: broadening participation, Mandela Day Symposium at Nelson Mandela University, South Africa, July 18, 2024
13. Spin crossover molecules for low power nonvolatile memory? Joint USA-European Symposium on ML, Simulations for ultra-low-power materials and devices, Spetses, Greece, July 7-13, 2024
14. Tuning the local environment of novel materials for a sustainable future, Interface Science Seminar, Fritz Haber Institute, Berlin, July 2, 2024
15. Tuning the local environment of novel materials for a sustainable future, GDCh Colloquium, Carl von Ossietzky Universität Oldenburg, June 27, 2024
16. Molecular Structures on Surfaces: toward hybrid interfaces, Physics Seminar, University of Kassel, June 25, 2024
17. Ultrafast charge dynamics and optical response in 2D materials: interplay of excitons & phonons, LMCQM Seminar, Universität Bremen, June 20, 2024
18. Designing novel materials for energy and quantum information, UCF NSF REU in Research in Materials for Energy Needs, May 21, 2024 (over zoom from Germany)
19. Excited state charge dynamics in 2D materials: interplay of excitons & phonons, Dynano-Seminar, Universität Oldenburg, May 15, 2024
20. *Ab initio* analysis of charges, excitons & phonons in 2D materials, Donostia International Physics Center, San Sebastian, March 26, 2024
21. "Diversity Matters – some strategies that could broaden participation," Donostia International Physics Center, March 22, 2023
22. The quest for spin crossover molecules for low power nonvolatile memory, APS March Meeting, Minneapolis, March 4-8, 2024. Invited talk at DCOMP Focus Session
23. Restructuring of a Physics Department with a little help from APS Bridge and PhysTEC Programs, APS March Meeting, Minneapolis, March 4-8, 2024. Invited talk at Forum on Education Symposium

24. Some strategies for strengthening pedagogical content knowledge of science teachers in Karachi, APS March Meeting, Minneapolis, March 4-8, 2024. Invited talk at Forum on International Physics Symposium
25. *Ab initio* analysis of the properties of excitons, Donostia International Physics Center, San Sebastian, February 29, 2024
26. "Engaging & Serving the International Community," Annual Leadership Meeting, American Physical Society, January 27-29, 2024
27. Enhancements in the implicit solvent model for simulations of the electrochemical environment for CO_2RR, CECAM Workshop on Atomistic Modeling of the liquid –solid interface, Lorentz Center, Leiden, January 8-12, 2024

2023

28. "Intriguing optical and chemical properties of 2D Materials: insights from theory and experiments" Festkoerperphysik Seminar, Ruhr Universität Bochum, November 24, 2023
29. Excited State Charge Dynamics and Optical Response of 2D materials: Role of Phonons, SMS 2023 & GIMRT User Meeting, November 20-22, 2023, Sendai, Japan,
30. Charge dynamics and optical response in 2D materials: interplay of excitons and phonons, Theoretical Physik Seminar, Universität Duisburg-Essen, November 17, 2023
31. Ultrafast charge dynamics and optical response in 2D materials: interplay of excitons and phonons, Physik Kolloquium, Universität Duisburg-Essen, October 25, 2023
32. Confinement Induced Enhanced Reactivity of Single Atom Catalysts, 796. WE-Heraeus-Seminar, Photoinduced, Charge-Driven, and Molecular Processes, September 24-28, 2023
33. Ultrafast charge dynamics and optical response in 2D materials: interplay of excitons and phonons, Applied Physics Seminar, Aalto University, September 8, 2023
34. Defected 2D Materials & Single Atoms on Oxides: possible catalysts for a sustainable future, ECOSS 36 Mini Symposium: Reactions on 2D Materials & Oxide Surfaces, Lodz, Poland, August 28-31, 2023
35. Designing catalysts for CO_2 conversion & molecules for spintronics: Can ML help? Spetses Symposium, Spetses, Greece, July 9-14, 2023
36. Theory, Modeling & Simulation of Reaction Mechanisms – part 2, LLNL Computational Chemistry & Materials Science Summer Institute, June 26-27, 2023
37. Theory, Modeling & Simulation of Reaction Mechanisms, LLNL Computational Chemistry & Materials Science Summer Institute, June 26-27, 2023
38. "Transient current calculations in spin-entangled systems: limitations of NEGF and possible advantage of TDDFT," M2QM All Hands Meeting, May 25, 2023
39. "2D materials for a sustainable future – the importance of being defected," Weed Distinguished Lecture, Chemistry-Biochemistry Department, University of Arizona, April 19, 2023.
40. "Organic - 2D Hybrid Materials – promises and challenges," Mini symposium, Chemistry-Biochemistry Department, University of Arizona, April 18, 2023.
41. "Defect, single atoms, other inhomogeneities that dictate the nature of the active site," Keynote talk, ACS Spring 2023 Symposium, Indianapolis, March 26-30, 2023.
42. "Essentials of the UCF-APS Bridge Program," IGEN Annual Meeting, Las Vegas, March 4, 2023
43. "APS Professional Skills Seminar," Conference for Undergraduate Women in Physics, UCF, January 20-22, 2023.

2022

44. "When Confinement becomes a virtue and novel chemical properties emerge," GDCh Colloquium, Bochum, December 1, 2022

45. Importance of being imperfect: Defect laden 2D Materials for a Sustainable Future," Physics Colloquium, Stoney Brook, October 25, 2022
46. "Diversity Matters – a glimpse at the UCF-APS Bridge to PhD," Advanced Photon Source, Argonne National Laboratory, October 20, 2022
47. "Defect laden 2D Materials for a Sustainable Future – from CO_2 conversion to single photon emission," RTG Colloquium, Ruhr Universität Bochum, October 11, 2022
48. "Computational Catalyst Design Methodology," Methodology Lecture, Ruhr-Universität Bochum, October 11, 2022
49. "Defect laden 2D Materials for a Sustainable Future – from CO_2 conversion to single photon emission," Physics Colloquium, University of Missouri - Columbia, September 26, 2022
50. "Defect mediated catalytic activity of 2D materials: MoS_2 and *h*-BN," 22nd International Vacuum Congress (IVC 22), Sapporo, Japan, September 12-16, 2022
51. "Exploiting defects in 2D Materials for a Sustainable Future – theory meets experiments," Palestinian Conference on Modern Trends in Mathematics and Physics (PCMTMP VII) Birzeit, July 30, 2022
52. "Most chemistry is local! Toward designing novel nanocatalysts with desired selectivity," Chemistry Colloquium, Carl von Ossietzky Universität Oldenburg, August 8, 2022
53. "Defect mediated catalytic activity of 2D materials: MoS2 and h-BN," Physical Chemistry Seminar, Justus Liebig Universität Giessen, July 22, 2022.
54. "Theoretical methods to explore the electronic structure of catalytic material and of reactions," PECASE22, San Sebastian, June 20-23, 2022.
55. "Quest for Transferable Neural Network Interatomic Potentials: success for Si(100), still looking for *h*-BN," Spetses Symposium on Deep Learning in Material Science, June 5-10, 2022
56. "An *Ab initio* Tool for Uncovering the Ultrafast Response of Functional Correlated Electron Materials," ES22 Electronic Structure 22, Columbia University, June 1-3, 2022
57. "Diversity Matters – a glimpse at two programs that have helped UCF-Physics: APS/IGEN Bridge to PhD and PhysTEC," April 22, 2022.
58. 2D Materials for a Sustainable Future – when imperfection reigns, Physics Colloquium, Penn State University, April 21, 2022.
59. Exploiting defects in 2D Materials for a Sustainable Future – when theory meets experiment," University of Texas Rio Grande Valley, April 8, 2022.
60. "Defect-laden 2D Materials for Syn Gas Conversion to Value-added Products," Argonne National Laboratory, March 23, 2022.
61. "Syngas molecules as probes of defects in 2D *h*- BN: their adsorption, vibrations & chemical reactions," From Surface Science to Catalysis Science Symposium, American Chemical Society, March 20-24, 2022, San Diego, CA.
62. "Single atom catalyst Pt_1/ZnO for methanol partial oxidation: insights into reaction mechanisms from DFT and experiments," Symposium to honor Miquel Salmeron, American Chemical Society, March 20-24, 2022, San Diego, CA.
63. "Surviving Graduate Studies - Diversity Matters," March Meeting, American Physical Society, March 12-16, 2022, Chicago.
64. "Designing Novel Materials for Energy & Quantum Information," Salam Day Lecture, Center for Physics Education, Karachi, Pakistan, January 29, 2022 (via ZOOM).
65. "The role of defects in emergent properties of 2D materials: MoS_2 and *h*-BN," Surface Science Discussions 2022, January 11-12, 2022, Poznan Poland (Online Edition).

2021

66. "An *Ab initio* Tool for Uncovering the Ultrafast Response of Functional Correlated Electron Materials," MRS Fall Meeting, Boston (mixed mode), Nov 29 –Dec 8, 2021.
67. "Diversity Matters: APS/IGEN Bridge to PhD," DOE Theoretical Condensed Matter Physics, PI Meeting, October 26, 2021 (via ZOOM).
68. "Tuning Properties of 2D Materials for a Sustainable Future, ICAPE 2021, September 16-17, 2021, NED College of Engineering, Karachi (via ZOOM).
69. "2D Materials for a sustainable future: prospects through intertwining theory with experiment," SUNCAT Summer Workshop, Stanford University, August 16-19, 2021 (via ZOOM).
70. "Tuning properties 2D materials for a Sustainable Future: from catalysis to single photon emission," Dhaka University Centennial Celebration, July 10, 2021 (via ZOOM).
71. "Two-Dimensional Folding of Polypeptides into Molecular Nanostructures," International Biophysics Workshop, Lahore University of Management Science (LUMS), March 25, 2021 (via ZOOM).
72. "Science in Confinement: From Surface Science to Nanoscience to 2D Materials," set of 10 lectures, Ruhr-Universität Bochum Mercator Fellow Lecture Series, March 2 – April 6, 2021 (via ZOOM).
73. "Polypeptide nanostructures at surfaces," International Biophysics Workshop, Lahore University of Management Sciences, Pakistan, March 25, 2021 (via ZOOM).
74. "The Self Learning Kinetic Monte Carlo (SLKMC) method augmented with data analytics for adatom-island diffusion on surfaces," APS March Meeting, March 15-19, 2021 (virtual).
75. "Defect-laden 2D materials for conversion of syn gas to higher alcohols: insights from theory and experiments," UCF-CECS Lunch Seminar Series, February 5, 2021 (via ZOOM).

2020

76. "Navigating scientific careers in the US – perspective from a woman academic," Pakistani Biophysicist Association, December 12, 2020 (via ZOOM).
77. "Modeling functional low dimensional materials," Universität Oldenburg, Germany, November 4, 2020 (via ZOOM).
78. "Women in Physics – how to make it not so few," Webinar on Women in Physics in the Developing World, Islamic University of Bahawalpur, Pakistan, October 19, 2020 (via ZOOM)
79. "Tuning properties 2D materials: from catalysis to single photon emission," Material Science Research Lecture Series, Caltech, October 14, 2020 (Webinar).
80. "Preferential CO_2 reduction to formic acid or methanol on defect laden single-layer *h*-BN," ACS CATL ChemistsLive Event, Sept 25, 2020; invited speaker and panelist (via ZOOM)
81. "Activating 2D materials for CO_2 and CO hydrogenation to higher alcohols: predictive modeling meets experiments," Mechanical & Aerospace Engineering Seminar Series, UCF, September 18, 2020 (via ZOOM)
82. "Defect-laden 2D materials for syn gas to higher alcohols: insights from theory & experiments," Catalysis Theory Virtua; Seminar Series, Denmark Technical University, September 3, 2020.
83. "Preferential CO_2 reduction to formic acid or methanol on defect laden single-layer *h*-BN," ACS Fall 2020 Virtual Meeting and Exposition, August 17-20, 2020 (video for presentation on demand).
84. "Single-molecule magnet for molecular electronics," EFRC-M2QM – Thin Film Discussion Group, May 15, 2020 (presented via ZOOM).
85. "Activating single-layer MoS_2 for conversion of syn gas to higher alcohols: insights from theory," ACS 2020 Spring Annual Meeting, March 21-26, 2020, Philadelphia, (presented electronically).

86. "Single-Molecule Magnets on Two Dimensional Materials: insights from ab initio calculations," MAGNA 2020, St. Simon Island, February 21-24, 2020.
87. "APS Bridge Site at UCF: background & some highlights," Conference for Undergraduate Women in Physics, University of Oklahoma, Norman, January 17-19, 2020. (Plenary talk)
88. "Modelling functional low dimensional materials," Conference for Undergraduate Women in Physics, University of Oklahoma, Norman, January 17-19, 2020.

2019

89. "Tuning properties of 2D materials: from catalytic activity to single photon emission," Computational Material Design Symposium, Quaid-e-Azam University, Islamabad, Pakistan, December 20, 2019.
90. "Toward Efficient Methods for Generating Transferable Neural-Network Interatomic Potentials," Computational Material Design Symposium, Quaid-e-Azam University, Islamabad, Pakistan, December 20, 2019.
91. "Challenges for Young Women Embarking on a Career in Science," Organization for Women in Science in the Developing World (OWSD), Pakistan National Chapter, Karachi, December 17, 2019.
92. "Toward efficient methods for generating transferable artificial neural network interatomic potentials," Materials Research Society 2019 Fall Meeting, Boston, December 1-6, 2019.
93. "Beyond DFT Methods that Capture the Role of Electron Correlations: Ultrafast Demagnetization of Ni," 2nd Symposium on MGI and Exascale Computing Challenges, Spetses, Greece, June 16-21, 2019.
94. "Tuning properties of 2D materials: from catalytic activity to single photon emission," 9th International Workshop on Surface Physics, Trzebnica, Poland, 24-28 June 2019.
95. "Tuning properties of 2D materials: from catalytic activity to single photon emission," Seminar, Max Planck Institute for Solid State Physics, July 17, 2019.
96. "2D materials for conversion of syn gas to higher alcohols: the role of defects and dopants," 2019 Gordon Research Conference on Dynamics at Surfaces, Salve Regina University, Newport, Rhode Island, July 28 - August 2, 2019.
97. "Novel and technologically relevant properties of 2D materials," Quaid-e-Azam University, Islamabad, March 12, 2019.
98. "Tuning properties of 2D materials: old dog new tricks," Mini-Workshop in Computational Material Design, COMSATS University of Technology, Islamabad, March 11, 2019.
99. "Modern paradigms in research and education: active learning to interdisciplinary research," Einstein Symposium, NED College of Engineering, Karachi, March 14, 2019
100. "Old materials with novel properties: you can teach an old dog new tricks in the flatland," LIFE Program Plenary Talk, UCF, March 19, 2019.
101. "Self-Learning KMC for multiscale simulation of nanoscale diffusion," 258th ACS Annual Meeting, Orlando, March 31, 2019.
102. "Tuning properties of 2D materials: old dog new tricks," Physics Seminar, Chalmers University, Gothenburg, April 5, 2019
103. "Stabilization of SMMs: interplay of ligands and substrates," M2QM-All Hands Meeting, University of Florida, May 3-5, 2019.

2018

104. "Surfaces, interfaces, and catalysis: what can machine learning do? 2nd IMPRESS (Interfacing Machine Learning and Experimental Methods for Surface Structures) Workshop, Graz, Austria, July 11-13, 2018.
105. "Unraveling & manipulating properties of 2D materials: old stuff with new promises," AMOSS Workshop, University of Milan-Bicocca, November 23, 2018.
106. "Multiple excitations, excited states, and ultrafast charge dynamics in functional materials: theory meets experiments," Palestinian Conference VI, Tulkaram, August 5-8, 2018
107. "Manipulating properties of 2D materials: old stuff with new promises," Palestinian Conference VI, Tulkaram, August 5-8, 2018.
108. "Catalysts, ultrafast spin dynamics, MGI and all else," Symposium on MGI and Exascale Computing Challenges, Spetses, Greece, June 10-15, 2018.
109. "Manipulating properties of 2D materials: old stuff with new promises," Condensed Matter Physics Seminar, University of California, Davis, April 26, 2018.
110. "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.
111. "Tuning 2D materials MoS_2 and h-BN for hydrogenation reactions," 255thAnnual ACS Meeting, New Orleans, March 18-22, 2018.
112. "Supported Au nanoparticles: good for methanol decomposition or formation?" American Physical Society March Meeting, Los Angeles, March 5-8, 2018.
113. "2D Materials: old stuff, new promises, and my Miller time," Miller Institute Lunch Talk, University of California Berkeley, February 27, 2018.
114. "Nanomaterial pursuit 2018: Inclusive or exclusive?" 2018 Conference for Undergraduate Women in Physics, University of North Florida, January 12-14, 2018

2017

115. "Towards multi-scale modeling of thin film growth processes," Fall Meeting of Materials Research Society (MRS), Boston, Nov. 26 – Dec. 1, 2017.
116. "Tailoring Chemical & Optical Properties of 2D Materials," Chemical Physics Department Annual Workshop, Fritz Haber Institute, Doellensee, September 25-29, 2017.
117. "Rational Material Design for Energy Needs: theory and experiment working in tandem," Karachi University, August 30, 2017
118. "Rational Material Design for Energy Needs: Follow up Workshop, COMSATS Institute for Information Technology, Islamabad, August 29, 2017
119. "Manipulating Chemical Reactivity of MoS_2 and other 2D Materials," Telluride Workshop on Computational Chemistry, August 7-11, 2017, Telluride.
120. "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.
121. "2D Transition Metal Dichalcogenides: old materials with new promises," Gesselschaft Deutscher Chemiker (GdCH) Colloquium, Ruhr University Bochum, July 6, 2017.
122. "Tailoring optical & chemical properties of 2D transition metal dichalcogenides," Summer School on Surfaces & Interfaces, San Sebastian, June 19-23, 2017.
123. "2D Transition Metal Dichalcogenides: old materials with new promises," Center for Nanoscience, Universitat Autonoma Barcelona, June 16, 2017.

124. "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.
125. "Tuning chemical reactivity of MoS2 and other 2D materials," Department of Chemistry and Chemical Engineering Seminar, Aalto University, Finland, May15, 2017.
126. "Rational Designing of Chemical & Optical Properties of 2D Transition Metal Dichalcogenides," COMP Seminar, Department of Applied Physics, Aalto University, Finland, April 19, 2017
127. "Computational Design of Metal –Coordination Centers for Catalytic Applications," 253rd ACS Spring Meeting, San Francisco, April 2-6, 2017.
128. "Tailoring properties of 2D transition metal dichalcogenides: looking beyond graphene," TMS Annual Meeting, San Diego, February 26-March 2, 2017.
129. "Graduate program assessment," Graduate Education & APS Bridge Program Conference, College Park, Maryland, February 10-12, 2017 (panelist).
130. "Cultivating relationships with School of Education," PhysTEC Annual Meeting, Atlanta, February 16-18, 2017 (panelist).
131. "Rational design of functional 2D materials," Donostia International Physics Center, San Sebastian, Spain, January 9-31, 2017 (5 lectures).

2016

132. "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.
133. "On computational design of functional 2D transition metal dichalcogenides," Max Planck Institute Workshop (Abteilung Kern), Schloss Ringberg, Taegernsee, October 16-19, 2016.
134. "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)
135. "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.
136. "Passion for science," Materials Science Colloquium, University of Milan, Bicocca, Italy, September 22, 2016.
137. "Tailoring chemical and optical properties of 2D transition metal dichalcogenides," International Conference on Solid Films and Surfaces (ICSFS18), Chemnitz, August 28-September 2, 2016.
138. "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.
139. "Reaction mechanisms: interplay of thermodynamics and kinetics," 2016 DOE Catalysis Science PIs Meeting, Gaithersburg, June 21-24, 2016.
140. "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).
141. "Tailoring properties of 2D transition metal dichalcogenides: looking beyond graphene," Physics Colloquium, Oulu University, Finland, June 3, 2016.

142. "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.
143. "Tailoring Characteristics of Nanoparticles: size, shape, composition and environment matters," Institute of Physics Seminar, Aalto University, May 30, 2016.
144. "Can an everyday lubricant be a novel material?" Physics seminar, University of the West Indies, Barbados, May 13, 2016.
145. "Can an everyday lubricant be a novel material?" Condensed Matter Physics seminar, Virginia Tech University, May 4, 2016.
146. "Towards increasing diversity in the UCF Physics Department: course reforms and the APS Bridge Program," Virginia Tech University, May 4, 2016.
147. "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.
148. "Tailoring properties of single and bilayer layer transition metal dichalcogenides: looking beyond graphene," Texas State University Physics seminar, April 12, 2016.
149. "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.
150. "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.
151. "Working effectively with university administrators," PhysTEC Annual Meeting, March 11-13, 2016, Baltimore (invited panelist).
152. "Tailoring properties of single and bilayer layer transition metal dichalcogenides: looking beyond graphene," U of Virginia Physics Colloquium, February 12, 2016.
153. "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

154. "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.
155. "Tailoring properties of single layer MoS2: looking beyond graphene," 3rd Euro-Mediterranean Conference on Materials for Renewable Energy (EMCMRE), Marrakesh, November 2-6, 2015.
156. "Self-Learning Kinetic Monte Carlo method and its application to adatom-island diffusion and coarsening," MRS Fall Meeting, Boston, Nov. 30 – Dec. 4, 2015.
157. "Tailoring characteristics of nanoparticles: size, shape, composition and environment matters," 250th ACS Meeting, Boston, August 16-20, 2015.
158. "Tailoring properties of single layer MoS_2: looking beyond graphene," Experimental Physics Seminar, University of Marburg, April 29, 2015
159. Reactivity of oxide and sulfide supported metal nanoparticles: role of the interface," From Witches Caldron to Material Science, Goslar, April 29-30, 2015.
160. "Ultrafast orbital charge dynamics and metallic domain growth in monoclinic VO_2," MURI Workshop of Ultrafast Science, University of Central Florida, November 12-13, 2015.

161. First International School on Computational Material Design," set of three invited talks, COMSATS Institute of Information Technology, Islamabad, Pakistan, May 25-29, 2015.
162. "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.
163. "Managing Faculty/Difficult Conversations," Physics Department Chairs Conference," American Physical Society, College Park, MD, June 5-7, 2015.
164. "Nano DMFT + DFTM: development of techniques beyond DFT," DRC2015 Lake Arrowhead Conference on Materials Defect, June 7-12, 2015.

2014

165. "Tailoring properties of single layer MoS_2: looking beyond graphene," Seminar, Department of Material Science, University of Texas, Austin, May 21, 2014
166. "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.
167. "A Combined DFT+KMC Study of Selective Oxidation of NH_3 on rutile RuO_2(110) at Ambient Pressures," DOE Contractors Meeting, Annapolis, July 20-23, 2014 (invited poster).
168. "Reactivity of oxide and sulfide supported metal nanoparticles: role of the interface," 248th ACS Meeting, San Francisco, August 10-14, 2014.
169. "Single Layer MoS_2: 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).
170. "Tailoring properties of single layer MoS_2: looking beyond graphene," International Materials Research Symposium, Cancun, August 18-21, 2014.
171. "Reactivity of oxide and sulfide supported metal nanoparticles: role of the interface," CINVESTA, Merida, Mexico, August 22, 2014.
172. "Self Learning Kinetic Monte Carlo for epitaxial growth: can pattern recognition help us out?" Professor Vashishta Fest, USC, August 29, 2014.
173. "Exotic 2D Materials at the Frontiers of Nanoscience, "Science Café, UCF, September 18, 2014.
174. 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.
175. "Tuning properties of single-layer transition metal dichalcogenides," IUPAC NMS-X (Novel Materials Synthesis and Characterization Symposium), ZhengZhou, China, October 11-15, 2014.
176. "Adaptation of Dynamical Mean-Field Theory for Nanoscale Systems," Computational Condensed Matter Physics Symposium, Tokyo, Japan, Dec. 2-4, 2014.
177. "Vibrational dynamics and thermodynamics as measures of nanoparticles structure," 3rd International Workshop on Phonons, Krakow, Dec. 4-8, 2014.
178. "Challenges and Frontiers of Physics Research & Education," COMSTECH Science Advisory Workshop, Islamabad, Pakistan, December 22-24, 2014.
179. "Tailoring properties of single layer MoS_2: looking beyond graphene," Physics Colloquium, USC, Los Angeles, March 10, 2014.
180. "Manipulation of electronic and chemical properties of single layer MoS_2: insights from first principles calculations", 247th American Chemical Society, Dallas, March 16-20, 2014.
181. "Tuning optical properties of arrays of pure and doped metallic nano chains," 247th American Chemical Society, Dallas, March 16-20, 2014.

2013

182. "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.
183. "Manipulating electronic & chemical properties of single layer MoS_2," Donostia International Center for Physics, San Sebastian, June 19, 2013.
184. "Electronic and chemical properties of single layer MoS_2: insights from ab initio electronic structure calculations**,** Marseille, June 25, 2013
185. "Band gap engineering in transition metal dichalcogenides," University of Genova, Italy, June 27, 2013.
186. "Computational design of functional nanomaterials: no longer a fiction," University of North Florida, Jacksonville, September 26, 2013.
187. Selectivity and reactivity of oxide-supported nanoparticles: role of the interface, Surface Chemistry Seminar, University of Liverpool, November 15, 2013.
188. "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).
189. "A Combined DFT+KMC Study of Selective Oxidation of NH_3 on rutile RuO_2 (110) at Ambient Pressures," 246th American Chemical Society, Indianapolis, September 8 – 12, 2013.
190. "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.
191. "Predictive modeling of materials for energy related needs," 60th Annual Meeting of American Vacuum Society, October 28 –November 1, 2013, Long Beach.
192. "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.
193. "Manipulating Electronic & Chemical Properties of Single Layer MoS_2," EMN Meeting, Orlando, April 9-12, 2013.
194. "Transforming a Physics Department," invited panelist at the Spring PhysTEC Meeting, Baltimore, March 15-17, 2013
195. "Single layer MoS_2: a promising material for nanoscience & nanotechnology," 2nd Symposium on Nanoscience and Nanotehnology, CNyN-UNAM, Ensenada, Baja California, March 4-8, 2013.
196. "Single layer MoS_2: insights from theory into another wunder-material," 53rd Sanibel Symposium, St. Simons Islands, GA, Feb 18-22, 2013.
197. "Computational design of functional nanomaterials: no longer a fiction," Southeastern Undergraduate Women in Physics Conference, Orlando, Jan 18-20, 2013.

2012

198. "Selectivity and reactivity of oxide surfaces: insights from *ab initio* calculations," Chemistry Colloquium, University of Pennsylvania, December 6, 2012.
199. 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.
200. "Nanoscience and Nanotechnology: achievements &challenges," Plenary lecture, QAU-Tech, Workshop on Nanoscience and Nanotechnology, Quaid-e-Azam University, Islamabad, Pakistan, October 1-5, 2012.
201. "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.
202. Tuning optical properties of Au chains through transition metal atom doping," DOE Contractors

Meeting, Theoretical Condensed Matter Physics, Rockville, August 19-22, 2012.

203. "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
204. "Tuning optical properties of transition metal chains and their arrays," Third Palestinian Conference on Physics and Mathematics, Hebron, July 14 – 17, 2012.
205. 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
206. "Tuning optical, magnetic and other interesting properties of nanoalloys for energy applications," NanoMexico12, Puebla, June 11-15, 2012.
207. "Optical properties of nanoalloys," Department of Physics, Aalto University, Espoo, Finland, January 16, 2012.
208. "Selectivity and Reactivity of oxide surfaces: insights from ab initio calculations," Colloquium Chemical Engineering Department, U of Florida, Gainesville, February 12, 2012.
209. Factors controlling the selectivity of oxide surfaces: results from DFT and KMC, 243rd ACS Annual Meeting, San Diego, March 25-30, 2012
210. "Tuning optical and other amazing properties of nanoalloy," Workshop on Nanoalloys, Brno, Czech Republic, April 2-4, 2012.

2011

211. "Density Functional Theory Method and its Applications," Workshop at National Center for Physics, Islamabad, Pakistan, December 28 – January 3, 2011 (set of 8 lectures).
212. "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.
213. "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.
214. (presented by postdoc Dr. Turkowski).
215. "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.
216. "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.
217. "Nanoalloys: playing fields of Alchemists revisited and refined," Physics Colloquium, University of Missouri, Columbia, 12 September, 2011.
218. 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
219. "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
220. "Nanomaterials for solar cell applications," First Euro-Mediterranean Conference on Materials and Renewable Energies (EMCMRE-1)., November 21-25, 2011

2010

221. "When gold is not gold anymore: size, shape and environment matters," Physics Colloquium, Florida Institute of Technology, February 20, 2010
222. "Selectivity and reactivity of oxide surfaces: insights from theory and modeling," Annual meeting of American Vacuum Society, Florida Chapter, March 8-10, 2010, Orlando.
223. "Nanoalloys: Playing fields of Alchemists revisited and refined," Physics Colloquium, University of Florida, April 1, 2010.

224. "Diffusion of large Molecules on Metal Surfaces: insights from ab initio calculations," Multiscale Modeling of Chemical Processes (MUMO), Turku, Finland, May 12, 2010.
225. "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.
226. "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).
227. "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.
228. "Nanoscience for mankind,"Salam Memorial lecture, Nathiagali, Pakistan, June 28, 2010.
229. Three lectures on Computational Material Design at 35th International Nathiagali Summer College, June 28 – July 3, 2010.
230. "Nanomaterials for mankind: fact or fiction," International Conference on Nano-Materials and Renewable Energies, Safi, Morocco, July 5-8, 2010.
231. "Atomistic Studies of Diffusion on Surfaces," 14th Workshop on Dynamical Phenomena on Surfaces, Schloss Ringberg, July 18-21, 2010.
232. "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.
233. "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.
234. "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)
235. "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)
236. "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

237. "Nanoalloys: composition and local environment controlling properties," Bahauddin Zakia University, Multan, Jan 12, 2009.
238. "Science at the Nanoscale:Building the world atom by atom," Islamia University Bahawalpur, Jan 13, 2009
239. "Nanoscience and Nanopatterning", Discussion Leader, 2009 Chemical Reactions at Surfaces Gordon Research Conference, February 8 - 13, 2009, Ventura Beach.
240. "Nanoalloys: playing fields of Alchemists revisited and refined," Physics Colloquium, University of South Florida, February 20, 2009
241. "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
242. "Nanoalloys: playing fields of Alchemists revisited and refined," Physics Colloquium, University of West Florida, April 6, 2009
243. "Policy and Chair Responsibilities," Leadership Excellence for Academic Diversity (LEAD) Workshop, Fayetteville, Arkansas, June 21-23, 2009
244. "Nanopatterning and its theoretical underpinnings,"three lectures given at the 34th International Nathiagali Summer College, Pakistan, June 27 – July 4, 2009.
245. "Nanoalloys: playing fields of Alchemists revisited and refined," Seminar, Max Planck Institute fuer Festkorperforschung, Stuttgart, July 22, 2009

246. 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.
247. "Challenges in academia for women of color" Fifteenth Annual faculty Diversity Institute on Teaching and Mentoring, October 23, Arlington, Virginia
248. "*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.
249. "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
250. "High CO tolerance of Pt/Ru nanocatalyst: Insight from first principles calculations," Chalmers University, Goteborg, Sweden, Dec 14, 2009.

2008

251. "Senior Women in Physics: what the numbers tell us, "ADVANCE Workshop on Women in Science and Engineering, Kansas State University, February 16, 2008
252. "Factors controlling reactivity of surface oxides and other nanostructures," seminar, Dept. of Physics, Technical University of Denmark, Lyngby, Denmark, April 28, 2008
253. "Factors controlling reactivity of surface oxides and other nanostructures," seminar, Dept. of Physics, University of Aarhus, Denmark, April 30, 2008
254. "Some Ways in which Surface Oxides Facilitate or Hinder Reactions," seminar, Chemistry Department, Brook Haven National Laboratory, NY, March 26, 2008
255. "On Factors that may facilitate or hinder the Reactivity of Surface Oxides," Chemical Engineering Colloquium, University of South Florida, Tampa, April 20, 2008
256. "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.
257. "Structure, dynamics, and vibrational entropy of bimetallic nanoalloys," seminar, Institut für Festkorper Physik, Forschungszentrum-Karlsruhe, Germany, June 16, 2008.
258. Three lectures on "Computational methods for nanoscale material design," 33rd International Nathiagali Summer College, Pakistan, June 28 – July 5, 2008.
259. "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.
260. "Nanoalloys: playing fields of our fore-fathers "the Alchemists" revisited and refined," Physics Colloquium, University of Delaware, October 3, 2008
261. "Women of Color in Academia: way forward," 15th Institute on Teaching and Mentoring, Southern Regional Education Board, Tampa, Florida, October 26, 2008.
262. "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.
263. "Nanoalloys: playing fields of Alchemists revisited and refined," Physics Colloquium, Temple University, Philadelphia, December 1, 2008.

2007

264. "Fuel Cells: a theoretical perspective," 32nd International Nathiagali Summer College, Nathiagali, Pakistan, June 25-30, 2007.
265. "Fuel Cell Reactions: some basics of theoretical calculations," 32nd International Nathiagali Summer College, Nathiagali, Pakistan, June 25-30, 2007.

266. "Theoretical Understanding of Reactions in Fuel Cells," 32nd International Nathiagali Summer College, Nathiagali, Pakistan, June 25-30, 2007
267. "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.
268. "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.
269. "Electronic and Geometric Structure, and Thermodynamics of Ag-Cu Nanoalloys," Condensed Matter Physics Seminar, Catholic University, Santiago de Chile, December 4, 2007.
270. "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.
271. "Novel Properties of Alloy Nanoparticles," Inaugural Symposium, National Center for Physics, Islamabad, Pakistan, March 26-29, 2007.
272. "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

273. Sigma Xi Distinguished lecture, University of Maine, March 2006, "Science at the nanoscale: promising facts or fiction?"
274. "Computational material design: challenges and prospects," Physics Colloquium, University of Central Florida, April 1, 2006.
275. "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
276. Sigma Xi Distinguished Lecture "Science at the Nanoscale: Promising Facts or Fiction?" University of Colorado, April 17, 2006.
277. "Science at the Nanoscale: Building Functional Materials Atom by Atom," Physics Colloquium, University of New Mexico, April, 2006
278. "Periphery motion or collective diffusion: the case of adatom islands on metal surfaces," 232nd ACS Annual Meeting, San Francisco, November 2006
279. "Anharmonic effects at metal surfaces," Workshop on Surface Dynamics, Modena, July 2006.
280. "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
281. "Molecular dynamics simulation of surface melting and roughing transitions," Workshop on Computational Material Science, JNCASR, Bangalore, July 6-10, 2006
282. Three lectures on computational nanoscience at the International Nathiagali Summer College, July 2006.
283. "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.
284. "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

285. 3rd US – Africa MRS Meeting and Workshop on Nanoscience and Nanotechnology, Dec 6-10, 2005, Marrakesh, "Computational Nanoscience: designing materials atom by atom."
286. 55th Midwest Solid State Conference, October 8-9, Columbia, Missouri, "Cluster Diffusion and Coalescence on Metal Surfaces using a Self Learning Kinetic Mote Carlo Method."

287. Sigma Xi Distinguished lecture, University of Vermont, September 22, 2005, "Should we tell our daughters to become scientist?"
288. Sigma Xi Distinguished lecture, Norwich University, Vermont, September 21, 2005, "Science at the nanoscale: promising facts or fiction?"
289. 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."
290. Solid State Physics Seminar, University of Twente, Netherland, July 20, 2005, "Atomistic studies of cluster diffusion and coalescence on metal surfaces."
291. 30th International Nathiagali Summer College, Nathiagali, Pakistan, July 3-9, 2005, set of four lectures on "Theory and modeling of materials at the nanoscale."
292. Sigma Xi Distinguished lecture, University of Wisconsin-Fox Valley, May 9, 2005, "Should we tell our daughters to become scientist?"
293. Sigma Xi Distinguished lecture, University of Wisconsin-Oshkosh, May 8, 2005, "When gold is no longer gold: a peek at matters at the nanoscale."
294. Speaker at a Symposium on "Women Scientists on Gender, Race, and Nationality," Massachusetts Institute of Technology, Boston, April 29-30, 2005.
295. Sigma Xi Distinguished lecture, Texas Christian University, April 22, 2005, "Science at the Nanoscale: promising facts or fiction?
296. Sigma Xi Annual Distinguished lecture, University of Puerto Rico, Mayaguez, April 21, 2005,"When gold is no longer gold: on tailoring properties of materials",
297. Sigma Xi Distinguished lecture, Emporia State University, Emporia, Kansas, April 16, 2005, "Science at the nanoscale: promising facts or fiction?"
298. Sigma Xi Distinguished lecture, Miami University, March 8, 2005, "Science at the nanoscale: promising facts or fiction?"
299. Sigma Xi Distinguished lecture, Corning Chapter, March 4, 2005, "Should we tell our daughters to become scientist?"
300. Colloquium, Corning Glass Industry, March 3, 2005, "Science at the Nanoscale: site selective properties controlling reactivity, morphology, and growth patterns on nanostructures."

2004

301. 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."
302. Sigma Xi Annual Distinguished Lecture, University of Kansas Medical Center, November 16, 2004, "Can nanotechnology keep us healthier?"
303. 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)."
304. Sigma Xi Distinguished Lecture, University of Missouri-Columbia, October 28, 2004,"Promises of Physics at the Nanoscale: fact or fiction?"
305. Sigma Xi Distinguished Lecture, Army Research Laboratory, Maryland, September 30, 2004, "Promises of Physics at the Nanoscale: fact or fiction?"
306. 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."
307. Annual Meeting of SPIE (Society of Optical Engineers), August 2-6, 2004, Denver, "Atomistic Modeling of Thin Film Growth Modes"
308. CMNRS Seminar, Marseille, July 19, 2004, "Site Selectivity in Chemical Reactions on Stepped Metal Surfaces."
309. Electrical Engineering Department Seminar, Lappeenranta University of Technology, Finland, June 29, 2004, "On theoretical measures of the reactivity of metal surfaces."

310. Fysik Laboratory Seminar, Helsinki University of Technology, June 28, 2004, "Diffusion of Two dimensional Cu Clusters on Cu(111)."
311. Chemical Physics seminar, Fritz Haber Institute, MPG, Berlin, July 21, 2004, "On poisons and promoters: theoretical measures of reactivity of metal surfaces."
312. 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."
313. Workshop on Nanoscience and Nanotechnology, Islamabad, Pakistan, April 11-16, 2004, "Physics at the nanoscale: set of 3 lectures."
314. 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."
315. 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"
316. Physics Colloquium, Washington University, St. Louis, March 4, 2004, "Physics at the nanoscale: where is the beef?"

2003

317. American Chemical Society, Annual Meeting, New Orleans, March 23-27, 2003, "On surfaces and nanostructures: under-coordination controlling the chemistry."
318. International Workshop on Surface Physics, Worslaw, Poland, September 12-15, 2003, "Site selectivity in chemisorption on metal surfaces: on poisons and promoters."
319. 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)."
320. University of Toledo, Physics Colloquium, November 20, 2003, "Physics at the Nanoscale: promising fact or fiction?"
321. 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."
322. Department of Applied Physics, Chalmers University of Technology, Goteborg, Sweden, May 22, 2003, "Role of undercoordination in determining the chemical reactivity of vicinal surfaces."
323. Laboratory of Physics Seminar, Helsinki University of Technology, June 16, 2003, "Optical Recognition of Steps on Metal Surfaces."
324. Department of Physics, Oulu University, Oulu, Finland, June 19, 2003, "On Poisons and Promoters on Stepped Pd Surfaces."
325. 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."
326. 28th International Nathiagali Summer College, Pakistan, June 24 – July 1, 2003 "Computational Techniques in Nanoscience and their Applications."

2002

327. Department of Chemistry, University of California, Riverside, December, 2002, "Role of under-coordinated sites in chemisorption and surface stability."
328. Department of Physics, University of Kansas, Lawrence, December, 2002, "Are we sacrificing science by jumping on the nano-bandwagon?"
329. Department of Physics, University of Rochester, Rochester, November, 2002, "Physics at the nanoscale: promising fact or fiction?"
330. Fritz Haber Institut, Berlin, July, 2002, "Does the corner kick control the game or is it the local coordination?"

331. Karachi University Colloquium, January 2002, "Challenges and opportunities in physics education." 27th International Nathiagali Summer College

2001

332. Department of Physics, Technical University of Denmark, January 19, 2001, "Vibrational Dynamics and Thermodynamics of Surfaces and Nanostructures".
333. NSF's Workshop on Partners in Nanotechnology, January 28-29, 2001, "Evolution of Nanoscale Film Morphology."
334. Ioffe Institute for Physics, Leningrad, Russia, April 17, 2001, "Finite Temperature Studies of Surfaces and Nanostructures".
335. Institute for Microelectronics, Yaroslavl, Russia, April 19, 2001, "Atomistic Studies of Epitaxial Growth on Metal Surfaces".
336. Department of Physics, Chalmers University, Goteborg, Sweden, May 11, 2001, "Self diffusion of Adatoms and Vacancies of Metal Surfaces: Paths, Processes and Diffusion Prefactors"
337. Physik Institut der Universitaet Zuerich, May 17, 2001, "Vibrational Dynamics and Thermodynamics of Surfaces and Nanostructures".
338. Series of 4 lectures on "Theoretical Methods for Calculating Finite Temperature Properties of Surfaces and Nanostructures", Fritz Haber Insitute, Berlin, May, 2001.
339. Annual Meeting of Alexander von Humboldt Foundation, June 2001, Berlin, "AvH Fellowship, AvH Forschungspreis, where do we go from here?"
340. Tenth Workshop on Dynamics at Surfaces, El Escorial, Spain, June 13-16, "Anharmonic Effects at Surfaces: temperature dependence of surface phonon linewidths."
341. 26th International Nathiagali Summer School, Nathiagali, Pakistan, June 26-July 5, 2001;
342. four lectures on "Microscopic Processes Responsible for Thin Film Growth."
343. Workshop on Characteristics of Stepped Cu Surfaces, University of Erlangen-Nuernberg, July 22-23, "Dynamics and Thermodynamics of Stepped Cu Surfaces".
344. Physik Department T30, Technische Universitaet Muenchen, July 24, 2001, "Novel properties of nanostructures: results of microscopic studies".

2000

345. 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."
346. 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."
347. 25th International Nathiagali Summer School, Nathiagali, Pakistan, June 26-July 5, 2000; three lectures on Nanotribology.
348. Laboratory of Physics Seminar, Helsinki University of Technology, September 19, 2000, "Thermodynamics of Nanocrystals."

RESEARCH SUMMARY

Rahman's primary interest is in understanding factors that govern novel properties (optical, magnetic, chemical, vibrational) of nanoscale materials in complex environments, to develop rules and guidelines for the rational design of these materials for a variety of applications, in a bottom-up approach. Since her focus is on relating fundamental science to functionality, she strives to make her theoretical and computational framework relevant to real-time experimental conditions. She works closely with experimentalists both to validate her predictions and to facilitate the rationalization of their experimental observations.

Her work attempts to address some of challenges faced by modern computational techniques based on *ab initio* electronic structure calculations: 1) reliable description of optical and magnetic properties of nanomaterials, particularly their response to external fields, 2) accurate inclusion of electron correlations; 3) accurate determination of diffusion/reaction pathways and rates; 4) determination of far from equilibrium behaviors in response to external perturbations; 5) multiscale modeling for passage of knowledge obtained at the microscopic level to predicting material behavior at higher levels. Considerations of issues such as stability of model systems, their structural transformation in operando, and the role of defects are central to Rahman's theoretical and computational framework. Competing effects of kinetics and thermodynamics and bridging of pressure, temperature and material gaps are also part of her scientific approach.

Theoretical & computational framework for understanding phenomena at the nanoscale

Rahman has established a state-of-the-art computational laboratory for simulating, understanding, and predicting properties of nanomaterials in complex environments. For this purpose, her group has adopted, developed and implemented accurate and efficient codes that extend beyond the standard. Building on density functional theory (DFT) her techniques accurately represent excited states, bound excitations (excitons, trion, etc.), correlated electrons, and far from equilibrium phenomena, through optimized variations of density-matrix based TDDFT [and dynamical mean-field theory (DMFT) [136,163]. The TDDFT+DMFT [91,58]], approach is a breakthrough for computationally feasible calculations of the properties of correlated electron systems and their response to ultrafast probes. Furthermore, through application of data science, she has advanced kinetic Monte Carlo (KMC) methods to overcome their incompleteness and empower predictability in the simulations [219,207,154]. Recently, her group has developed codes employing grand canonical DFT, *ab initio* molecular dynamics, and an efficient explicit-implicit solvent model for *ab initio* calculations of electrochemical environments [1].

Below are some highlights of Rahman's research accomplishments. Citation numbers as in the publication list that follows.

A. Understanding the role of surface vibrations

Rahman's career in materials physics began with her theoretical work in surface phonon dispersion which allowed several prominent experimentalists in the field to obtain insights into the effect of surface phonons on a variety of surface phenomena. Her work was particularly helpful to experimentalists working with electron energy loss spectroscopy and helium atom surface scattering in their pioneering measurements of the dispersion of surface phonons on metal surfaces (with and without adsorbates) [315,327,306,310].

She has contributed significantly to understanding the role played by surface vibrations in determining the thermodynamics of confined systems such as surfaces [270] nanoparticles [228]. In a first theoretical investigations [266] of the vibrational modes of nanoparticles, Rahman's group predicted the enhancement of the density of states of modes with frequencies that lie in the lower end of the vibrational spectrum, as well as the emergence of new modes with frequencies above the bulk band. Both predictions have been confirmed by experiments. More importantly the linear variation of the density of states with energy, at low frequencies leads to large deviations of the heat capacity of nanoparticles from the bulk T^3 rule.
An important consequence of the above work is that the bulk concept of Debye temperature cannot be applied to nanoparticles unless their size is larger (> 3-4 nm) than that predicted by Rahman et al. The citation below elaborates further on the novel vibrational dynamics of nanoparticles that make them so distinct from their bulk counterparts [146].

Her work helps extract the role of vibrational entropy in growth processes, as it may affect the characteristics of atom and atomic-cluster diffusion on surfaces. Her work points to the dependence of the diffusion pre-exponential factors on vibrational entropy [262,47]. Since the latter depends on the local atomic environment and local confinement, her work provides a path to controlling the diffusion of adatom and

molecules on surfaces. Rahman was the first to establish the role of atomic/molecular vibrations in determining reaction and diffusion rates, providing a pathway for accurate determination of diffusion prefactors, as they may play pivotal roles in surface diffusion [271].

B. The implications of anharmonic effects on surfaces

Using a combination of molecular dynamics and lattice dynamics, Rahman's group has provided insights into the role that anharmonic effects play in surface phenomena [290]. They have provided guidelines for the validity of the quasiharmonic approximation in the interpretation of experimental data [253]. These calculations of phone linewidths and surface thermal expansion helped interpret experimental data without the deficiency of simple DFT-based calculational based that had earlier led to erroneous conclusions.

C. Novel phenomena on surfaces and interfaces: adsorption, diffusion, reaction

A significant effort in Rahman's group is on understanding microscopic processes that are responsible for a variety of phenomena on solid surfaces. Insights from electronic structure calculations of the molecule-surface interactions [216] led to the designing of a "cargo" bearing "walking molecule" and provided the rationale for experimental observations in collaborator Bartels (UC Riverside) laboratory. This Science article (January 2007) received world-wide publicity because of implications in drug-delivery [194].

In early efforts to understand and predict the descriptors of chemical reactivity Rahman drew an important conclusion from *ab initio* studies of methanol decomposition on oxide-supported Au nanoparticles [132] that the activity came from atomic sites at the Au-titania interface, because of charge transfer. This points to ways in which the characteristics of the molecule-interface system could be manipulated for functionalities such catalysts. Her body of recent work on single atom catalysts (SAC) in which transition metal atoms secured on metal oxide surfaces display selectivity in reaction products, builds on the above and provides a fundamental understanding of the local atomic environment and electronic structure that is responsible for novel properties of these materials, as demonstrated so eloquently in the Nature Communication publication [29]. She has also investigated the role of defects, ligands [26,13], and the nature of the elemental metal [57] and the oxide support [81,9] to figure out the design rules for the accelerating her theory-led discovery of these novel materials.

Rahman's versatility in extracting physical insights from electronic structure calculations supplemented by high powered experimental observation (in this case scanning tunneling microscopy) is further evident in a recent publication on a hybrid molecular-metal interface which shows the formation of a Kagome-type lattice induced by the interaction of the molecular overlayer with the Au surface states [6].

D. Understanding growth and morphological evolution

Her development of an accelerated on-lattice [219] and off-lattice [176,148] "self-learning" kinetic Monte Carlo methods are milestones in realistic simulations of growth modes of thin films and nanoparticles on substrates. Through a self-created database of events and machine learning, model systems are allowed to evolve on their own accord (without a priori bias) revealing rate-determining atomistic mechanisms and making rare events tractable -- a giant step towards the grand challenge of multi-scale modeling. By providing a strategy to address the "completeness" limitation of standard KMC (which depends on an *a priori* list of atomistic processes (reaction pathways) that moving entities are expected to undergo), Rahman's approach can predict stable islands sizes, growth patterns and morphological evolutions in phenomenon such as thin film growth [125]. Through combination of *ab initio* methods based on DFT for system energetics and vibrational dynamics and KMC for system kinetics, Rahman's group is able to carry out reliable and robust multiscale modeling (mesoscopic length scales and time scale of seconds) a large number of surface phenomena [156,175]. Such predictive power does not exist with standard KMC.

E. Prediction of reaction rates, reaction intermediates and turnover frequencies

Her work in catalysis predicts mechanisms underlying the key microscopic processes responsible for molecular/atomic adsorption, dissociation, desorption, and diffusion, which are the necessary steps in chemical reaction. Her methodology which combines DFT and KMC also undertakes determination of the rates of chemical reactions and turn over frequencies, which allow direct comparisons with experimental observations, unlike what is possible from calculations of just the process energetics (using DFT). For example, her proposed framework for explaining reaction selectivity in ammonia oxidation on ruthenium-dioxide surface, observed by Ertl's group, paved the way for accurate computation of reaction rates from information at the microscopic level [160]. It also helped explain why reaction rates obtained under industrial conditions may not be the same as those obtained in controlled ultrahigh vacuum [111].

F. Novel chemical and optical properties of 2D materials

Her work in 2D transition metal dichalcogenides is multifaceted and done in collaboration with several experimental groups. Most outstanding is the prediction of the *chemical reactivity of vacancy-laden MoS_2*. Her groundbreaking work in 2014 showing electronic structural changes induced by defects in single layer MoS_2 may lead to catalytically active [113] have been confirmed in her collaborative work with experimentalists [62]. More dramatically her work on *defect-laden hexagonal boron nitride* which Rahman et al. show not only to be a good hydrogenation catalyst [100] but can also convert CO_2 to methanol [*42,2]*. This viability of a metal free catalyst for reactions of technological importance may be game changers. They also shine light on novel properties that emerge in reduced dimensions and in realistic systems with heterogeneous local atomic environments that Rahman investigates.

Rahman's recent work [92,119] using density matrix based TDDFT to examine the characteristics of the variety of excitons in 2D materials has provided the community with an accurate and computationally feasible ab initio method for calculating the binding energies of excitons, trions, and biexcitons with results that are in good agreement with experimental observations. The beauty of the methodology [17] is that it not restricted to calculations of the system energetics but also to its temporal evolution in response to an external perturbation. It also calculates the excitation spectrum – something typically not done in theoretical calculations. These enhancements in the methodology allow direct contact with experiments as is displayed in their recent work in which exciton-phonon interactions, and not just the usual electron-phonon interactions, when properly included in the calculated emission spectra account for the observed anomalous shift of the photoluminescence with Mo isotope mass [7]. The exposition of the role of electron exchange interactions in distinguishing the binding energy of the bright and dark exciton in single layer WSe2 is another achievement [17].

G. Tracing the role of electron correlations via response to ultrafast probes

Rahman and co-workers have developed a technique based on dynamical mean field theory (DMFT) and time dependent density functional theory (TDDFT) that allows them to include the effects of electron correlations in a reliable manner. Their work reveals that when such a system (with significant electron correlations) is optically excited, the signatures of exchange-correlation interaction are most consequential in first few femtoseconds of the excited states charge and spin dynamics and leads to interesting novel characteristics. With DMFT+TDDFT, Rahman has shed light on the role of electron correlations and memory effects on the demagnetization of Ni at the femtosecond timescale [58] that had remained a puzzle for 5 decades. This powerful and efficient technique has also provided an understanding, based on first principles, of the critical role of electron correlations and memory effects in the much-debated insulator to metal transition in VO_2 that has perplexed theorists for the past 50 years [55].

H. Insights into electrochemistry from ab initio methods beyond DFT

Rahman's physicist approach to exposes the microscopic mechanisms that control the electrochemical

conversion of carbon dioxide to value added products by developing computational techniques that replicate the challenging area of liquid-solid interfaces. The recent examination of the role of ammonium-based cations on CO_2 [1] is a masterpiece in exposing the physics of the electrochemical environment through techniques that engage grand canonical DFT and *ab initio* molecular dynamics together with strategies for explicit inclusion of the solvent that had been a challenge in the field.

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