Talat Shahnaz Rahman

Department of Physics
University of Central Florida
Orlando, FL 32816

(407) 823-1480
http://www.physics.ucf.edu/~talat
Email: talat.rahman@ucf.edu

Professional Preparation

Karachi University	Physics (Honors)	B. S. (highest distinction)	1969
Islamabad University	Physics	M. Phil	1970
University of Rochester	Physics	Ph. D	1977
University of California, Irvine	Surface Physics	Postdoc	1977 - 1979

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 - 2015 Distinguished Professor & 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

Some Recent Additional Appointments

Helene Lange Guest Professor, Carl von Ossietzky University Oldenburg, Germany, 2022 –
Senior Mercator Fellow, Ruhr University Bochum, Germany, 2020 -2022
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, Spain, 2016 - 2018 (Summers)
Visiting Scientist, Max Planck Institut für Festkörperforschung, Stuttgart, July, 2009-2015 (Summers)
Visiting University Professor, Helsinki University of Technology, Finland, Fall Semester 2000
Visiting Scientist, Fritz Haber Institute, MPG, Berlin, Spring Semester 2001, Summer 1998-2007.

Five Current Publications

1. E. Mishra, T. K. Ekanayaka, T. Panagiotakopoulos, D. Le, T. S. Rahman, P. Wang, K. A. McElveen, J. P. Phillips, M. Z. Zaz, S. Yazdani, A. T. N'Diaye, R. Y. Lai, R. Streubel, R. Cheng, M. Shatruk and P. A. Dowben "Electronic structure of cobalt valence tautomeric molecules in different environments," Nanoscale 15, 2044 (2023) https://doi.org/10.1039/d2nr06834f
2. T. Ekanayaka, T. Jiang, E. Delahaye, O. Perez, J-P Sutter, D. Le, A. T. N'Diaye, R. Streubel, T. S. Rahman, P. A. Dowben, "Evidence of Symmetry Breaking in a Gd_2 di-nuclear molecular polymer," Phys. Chem. Chem Phys (2023). https://doi.org/10.1039/D2CP03050K
3. J. Shi, V. Turkowski, and T. S. Rahman, "Dark exciton energy splitting in monolayer WSe2: insights from time-dependent density functional theory." Phys. Rev B 107, 155431 (2023). https://doi.org/10.1103/PhysRevB.107.155431
4. W. Tan, S. Xie, D. Le, W. Diao, M. Wang, K. Low, D. Austin, S. Hong, F. Gao, L. Dong, L. Ma, S. Ehrlich, T. S. Rahman, and F. Liu, "Fine-tuned local coordination environment of Pt single atoms on ceria controls catalytic reactivity" Nature Commun. **13**, 7070 (2022). https://doi.org/10.1038/s41467-022-34797-2
5. D. Le and T. S. Rahman, "On the role of metal cations in CO2 electroreduction," Nature Catalysis 5, 977 (2022) https://doi.org/10.1038/s41929-022-00876-2

Five Other Publications

1. E. D. Switzer, X-G. Zhang, and T. S. Rahman, "Anisotropy-exchange resonance as a mechanism for

entangled state switching, Phys. Rev. A 104, 052434 (2021); https://doi.org/10.1103/PhysRevA.104.052434

2. T. B. Rawal, S. R. Acharya, S. Hong, D. Le, Y. Tang, F. F. Tao, and T. S. Rahman, "High Catalytic Activity of $Pd_1/ZnO(10\bar{1}0)$ toward Methanol Partial Oxidation: A DFT+KMC study, ACS Catal. 8, 5553 (2018).
3. J. Pal, T. B. Rawal, M. Smerieri, S. Hong, M. Alatalo, L. Savio, L. Vattuone, T. S. Rahman, and M. Rocca, "Adatom extraction off pristine terraces by dissociative oxygen adsorption at metal surfaces: Combined STM and DFT investigation of O/Ag(110), " Phys. Rev. Lett. 118, 226101 (2017).
4. D. Le, T. B. Rawal, and T. S. Rahman, "Single-Layer MoS_2 with Sulfur-Vacancies: Structure and Catalytic Application," J. Phys. Chem. C 118, 5346 (2014).
5. S. Hong, A. Karim, T. S. Rahman, K. Jacobi, G. Ertl, "Selective Oxidation of Ammonia on $RuO_2(110)$: a combined DFT and KMC study," J. Catalysis **276**, 371 (2010).

Graduate Students mentored: PhD Thesis Committee Chair for:

1. Eric Switzer, PhD Summer 2023
2. Nasim Uddin, PhD Fall 2020
3. Tao Jiang, PhD Fall 2019
4. Zahra Hooshmand, PhD Fall 2018
5. Shree-Ram Acharya, PhD Spring 2018

Masters Students: Rainier Berkley, MS 2018; Andre Childs, MS 2018
Current PhD students at UCF: Theodoros Panagiotakopoulos, Bushra Ashraf, Dave Austin, John Janisch, Faiza Rubab.
Total Number of PhD Students Supervised over the course of career: 37.
Total Number of PhD Students graduated in past 7 years: 10.

Synergistic Activities

- My research group has established at UCF a modern, interdisciplinary computational framework for understanding and predicting properties of functional nanomaterials in complex environments. An outstanding contribution is the development of a technique combining time dependent density functional theory (TDDFT) and dynamical mean field theory (DMFT) that allows accurate determination of the role of electron correlations through the ultrafast response of the material to external fields. Another is the application of DFT and kinetic Monte Carlo (KMC) to reveal mechanisms that control chemical reactions of technological and societal importance.
- Our development of an accelerated "self-learning" kinetic Monte Carlo method is a milestone 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.
- For the American Vacuum Society as an Executive Comm. Member (2015-17) and chair of the Diversity and Inclusion Committee (2017-2021) organized workshops and helped create structures that promote an inclusive environment at annual meetings.
- As the Site Leader for the PhysTEC Comprehensive Site at UCF, whose goal is to increase the number of skilled physics teachers, helped UCF join the 5+ Club (producing 5 or more physics teachers in a year) and establish the Learning Assistant program at UCF; also led an NSF-supported pedagogy reform in introductory physics courses.
- Site Leader for UCF's APS-Bridge Program aimed at increasing the number of PhD students from Underrepresented Minority (URM) groups. This program has helped raise the number of URM physics graduate students at UCF to ~ 20% - the highest in the nation. Several have already graduated with a PhD and are successfully employed.
- As chair-elect APS Division of Computational Physics (DCOMP), organized 59 sessions at the APS 2023 March Meeting; currently (2023-24) as DCOMP chair organizing also international activities.