

**Amirkabir University of Technology  
(Tehran Polytechnic)**

# **AUT - DFG**

**Joint Matchmaking Webinar**

**April 2021**

# Keivan Aghababaei Samani

## Mahdi Hajihashemi

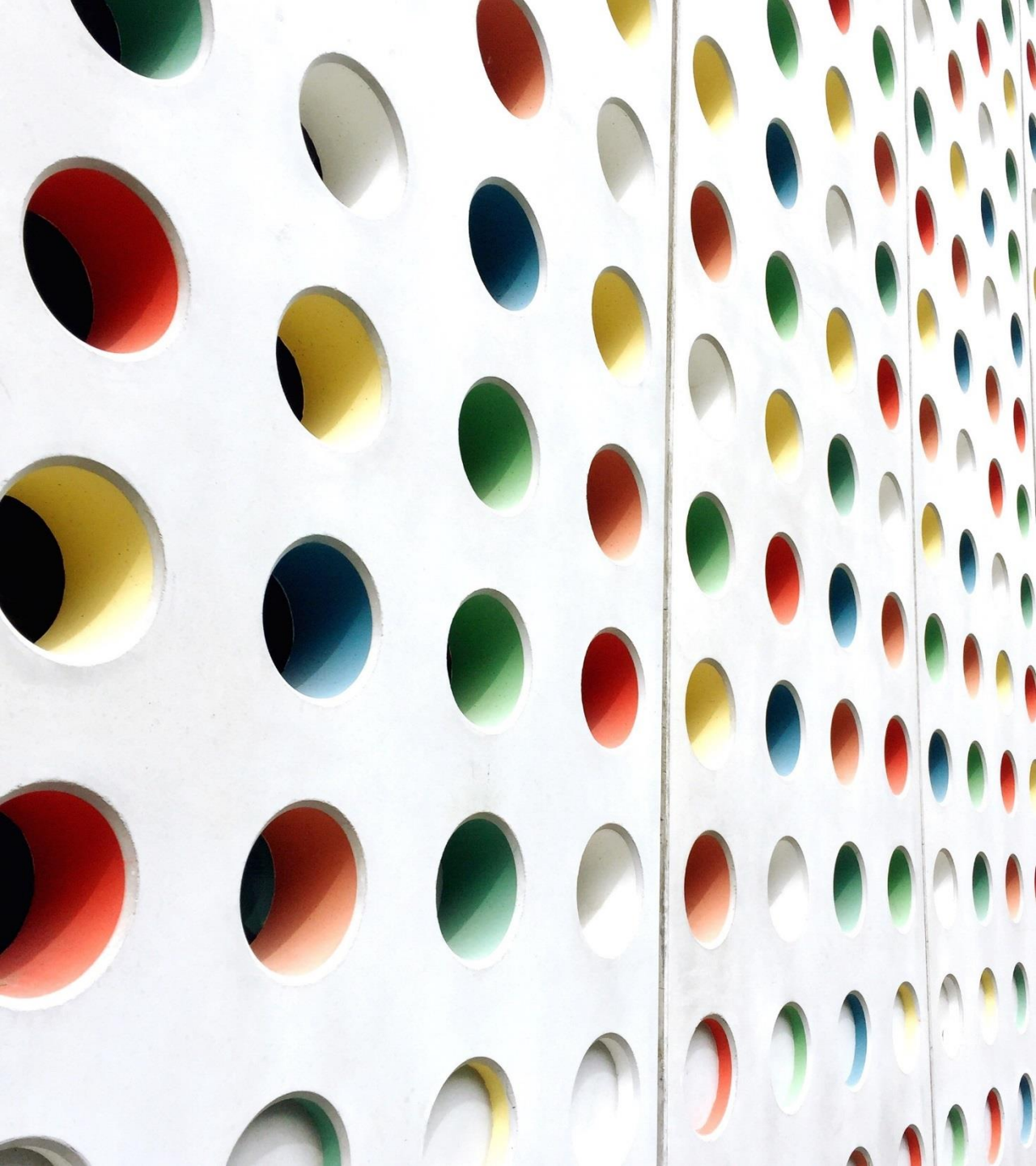
# Structure and dynamics of complex networks; Evolutionary dynamics on complex networks.

# Group Research/Industrial Projects

**Investigating fixation time and fixation probabilities of the Moran process on complex networks**

# Group Contact Information

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# Research Group CV

<b>Name:</b>	Maryam Mostajeran	
<b>Sex:</b>	Female	
<b>Nationality:</b>	Iranian	
<b>Languages:</b>	Persian (native) & English	
<b>Institution and department:</b>	Yazd University, Physics department	
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<b>Website :</b>	<a href="https://pws.yazd.ac.ir/mostajeran/">https://pws.yazd.ac.ir/mostajeran/</a>	

# Research Group CV (VISITING SCHOLAR:)

<b>Institute:</b>	National Synchrotron Radiation Center (NSRRC), Taiwan
<b>Period:</b>	23December 2006- 22December 2007
<b>Description:</b>	I attended in RF team, my research was dealing with multipacting phenomenon.
<b>Institute:</b>	ESS Proton linear accelerator, Uppsala, Sweden.
<b>Period:</b>	December 11-17, 2011.
<b>Description:</b>	I invited to visit there (RF team) and participated in the workshop.
<b>Institute:</b>	Rostock University, Germany
<b>Period:</b>	5 September – 5 October 2016, 22 July – 23 August 2017, 23 July-23 August 2018.
<b>Description:</b>	I invited to visit there and I joined with the group of General Electrical Engineering. My research was dealing with multipacting phenomenon



# Research Group Interest

Electromagnetic fields in Accelerator physics

Multipactor phenomenon

Uncertainty Quantification for Accelerator devices

Nonlinear systems

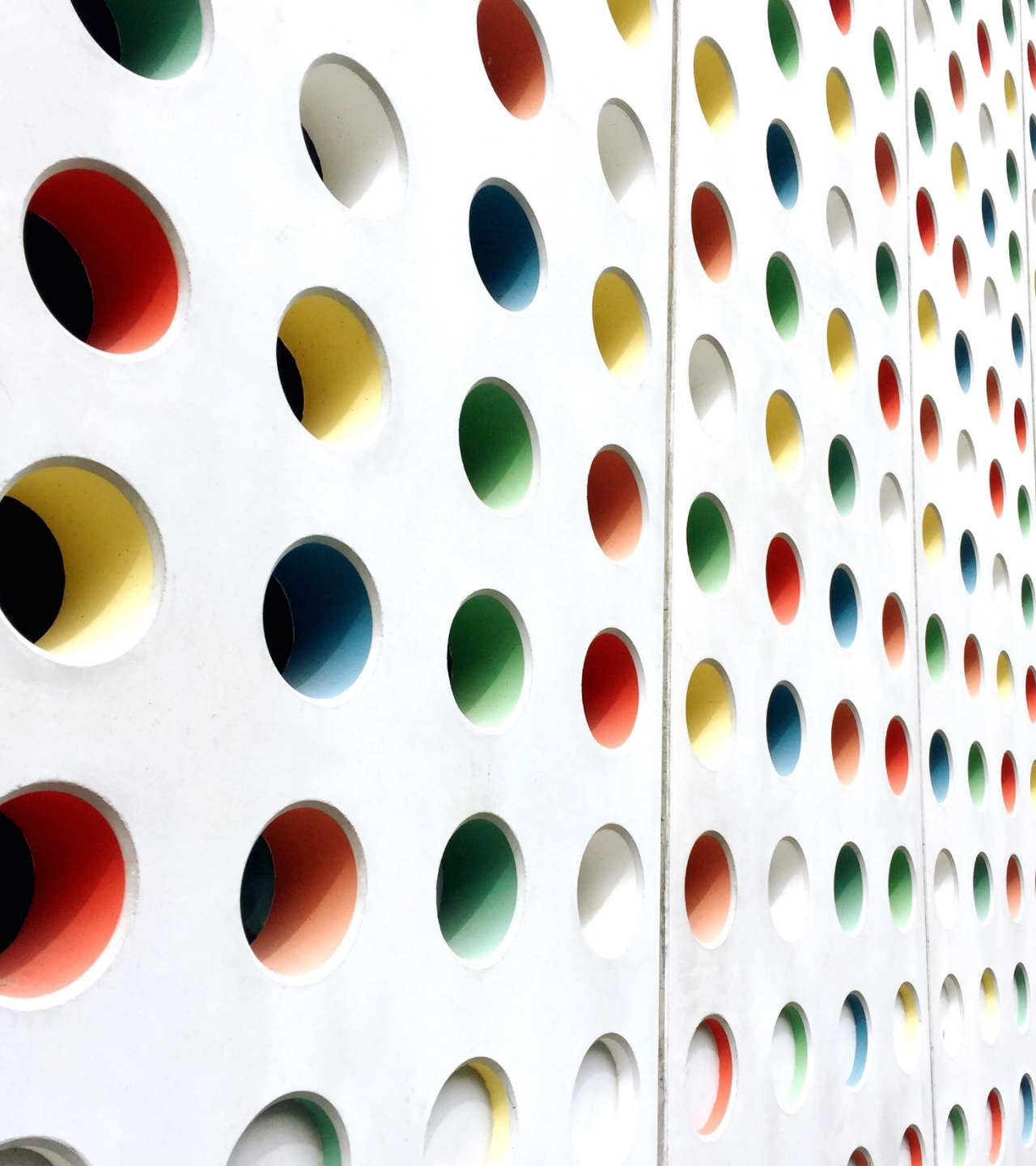
# Group Research/Industrial Projects

## International Project:

Funding for the Initiation of International Collaboration, supported by DFG, Germany, 2016.

## Out Put:

M. Mostajeran, E. T.Tulu. U. Van Rienien, “ Uncertainty in the multipactor threshold of isosceles triangular grooved surfaces based on polynomial chaos”, ” Nuclear Inst. and Methods in Physics Research, A 165001 (2021).



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# Research Group CV

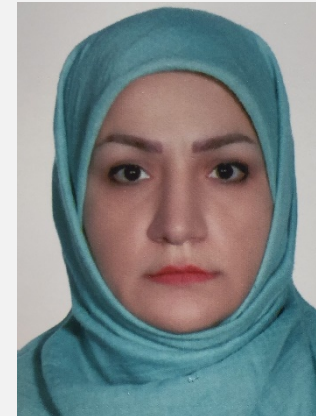
## Dr. Michael Fischer

- **10/2002 to 12/2007: University of Hamburg**  
Studies in Mineralogy  
Degree: Dipl.-Min.
- **01/2008 to 12/2011: University of Hamburg**  
PhD studies in Inorganic Chemistry  
Degree: Dr. rer. nat.
- **02/2012 to 01/2014: University College London**  
**Department of Chemistry**  
Postdoctoral scholar (DFG-funded)
- **Since 02/2014: University of Bremen**  
**Faculty of Geosciences**  
Independent researcher (third-party funded)  
within the **Crystallography group**



## Dr. Saeedeh Sarabadani Tafreshi

- **1998 to 2002 : Sharif University of Technology, Tehran, Iran**  
**Department of Chemistry**  
Degree: BSc in Applied Chemistry
- **2002 to 2005: Alzahra University, Tehran, Iran**  
**Department of Chemistry**  
Degree: MSc in Physical Chemistry
- **2011 to 2015: University College London,**  
**Department of Chemistry**  
Degree: PhD in Computational Chemistry
- **2017 to 2018 : Sharif University of Technology, Tehran, Iran**  
**Department of Physics**  
Post-doctoral researcher
- **Since 2018: Amirkabir University of Technology (Tehran Polytechnic),**  
**Chemistry Department**  
Assistant Professor



# Research Group Interest

## Dr. Michael Fischer

### Computational studies of porous materials

- Force field based simulations
- Density functional theory (DFT) calculations
- DFT-based molecular dynamics

### Zeolites

- Host-guest interactions
- Dynamics of framework atoms and extra-framework species
- Gas adsorption and separation
- Adsorption of organic pollutants

### Host-guest interactions in metal-organic frameworks

### Polymorphism and phase transitions in minerals and inorganic materials

## Dr. Saeedeh Sarabadani Tafreshi

Density functional theory (DFT) studies in the fields of:

- Heterogeneous catalysis
- Semiconductor heterogeneous photocatalysis
- Drug delivery
- Solar cell
- Fuel cell
- Lithium-ion batteries
- Hydrogen storage

# Group Research/Industrial Projects

## Dr. Michael Fischer

### Ongoing DFG project: *Beyond tetrahedral coordination in zeolite-type materials – A computational approach*

- Static and dynamic calculations on fluoride-containing all-silica zeolites
- Investigation of water adsorption in aluminophosphates and silicoaluminophosphates

### New DFG project (from 10/2021):

- Adsorption of emerging contaminants, especially pharmaceuticals, in zeolites

### Various research collaborations

- Department of Chemistry, University of Bremen (D)
- Mineralogical Institute, University of Hamburg (D)
- Max Planck Institute for Coal Research, Mülheim (D)
- Wrocław University of Science and Technology (Poland)
- CICECO/University of Aveiro (Portugal)

## Dr. Saeedeh Sarabadani Tafreshi

### Research projects:

- Computational study of CO<sub>2</sub> hydrogenation on the early transition metal carbide surfaces using DFT.
- First-principles study of optic and electronic study of earth alkaline metals doped formamidinium lead iodide perovskite.
- DFT study of phosphorene as a new drug-delivery system to nitrogen mustards chemotherapy drugs.
- Computational design of Trimetallic Borohydrides as new hydrogen storage materials.
- DFT calculations on hydrogenation of CO through Fischer-Tropsch synthesis in the presence of metal catalysts.
- Computational study of CO hydrogenation through Fischer-Tropsch synthesis over graphene oxide based catalysts using DFT.
- DFT study of CO hydrogenation on SiO<sub>2</sub> based catalysts.
- Computational study of CO<sub>2</sub> hydrogenation on two dimensional transition metal nitride surfaces using DFT.



# Group Supervised Labs

**Dr. Michael Fischer**

## **Computing facilities:**

- Access to local and regional (HLRN) high-performance computing facilities

## **Experimental facilities:**

- Within the Crystallography group: X-ray diffraction (powder, single crystal), thermoanalysis, microscopy
- Access to various other facilities within the University of Bremen via MAPEX Center for Materials and Processes

**Dr. Saeedeh Sarabadani Tafreshi**

## Computing facilities for doing DFT calculations:

- A supermicro server at AUT chemistry department
- Access to Parallel processing services center of AUT (HPCRC)
- Access to the Advanced Research Computing at Cardiff (ARCCA)
- Access to the departmental cluster ( ib-server) at UCL Chemistry Department



# Group Contact Information

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