

# بیست و سومین

# کنفرانس شیمی فیزیک انجمن شیمی ایران

۲۲ و ۲۳ دی ۱۴۰۰ کرمان، دانشگاه شهید باهنر



فاخره صبا

ای درخت پر ثمر بادت بهیچ  
ای خداوند هنر بادت بهیچ

فیسر سر جرم اتمی پور



مهندس علیرضا اتمی پور

باید امروز، فردا دیر است

سرینگار دانشگاه کرمان

23<sup>RD</sup>

Iranian Conference on Physical Chemistry

12-13-Jan 2022 – Shahid Bahonar University of Kerman

## محورهای کنفرانس

ترمودینامیک شیمیایی | سینتیک شیمیایی | ترمودینامیک آماری

شیمی کوانتومی | طیف سنجی مولکولی | الکتروشیمی

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برگزارکنندگان



SCAN ME

دبیرخانه کنفرانس: کرمان - بزرگراه امام خمینی - میدان پژوهش - دانشگاه شهید باهنر کرمان - بخش شیمی

تلفن تماس - واتس آپ:

۰۹۱۷۳۱۶۵۱۰۶

تلفن دبیرخانه: ۰۳۴-۳۱۳۲۲۱۲۶

وبسایت کنفرانس: [physchem23.uk.ac.ir](http://physchem23.uk.ac.ir)

ایمیل کنفرانس: [physchem23@conf.uk.ac.ir](mailto:physchem23@conf.uk.ac.ir)

▶ **The 23<sup>rd</sup> ICS Physical Chemistry Conference**



▶ **Chemistry Department, Faculty of science, Shahid Bahonar**

**University of Kerman**

▶ **Kerman, Iran**

▶ **12-13 Jan 2022**



▶ **Conference Program**



▶ **Dedicated to Alireza Afzalipour and Fakhreh Saba,**

▶ **The Founders of Kerman University**

# General Information

In order to attend the Conference virtually, it is required to install both Adobe Connect and Adobe Flash Player on your device.

Then, please take the following steps to enter the meeting:

1. Open the Adobe Connect,
2. Copy and paste the related link (for example, <http://physchem23.ir/main>), and then press the Continue button,
3. Type your name as a guest and enter the room.

Additionally, we should mention that

1. The details and related links of the Seminar programs can be seen at <https://physchem23.uk.ac.ir>
2. Invited Talks, Opening, Closing, Parallel Lectures are presented in Persian.
3. The duration of each Invited Talk is 50 minutes and 10 minutes for questions.
4. The duration of each Lecture is 15 minutes and 5 minutes for questions.
5. Posters are presented during the whole conference with Slideshow at [Link M](#).
6. The Opening and Closing will be at [link M](#).
7. The Invited Talks will be at links [T1](#) and [T2](#).
8. The Lectures will be at links [P1](#) and [P2](#).
9. The Break and Networking will be at [link B](#).
10. The Workshops will be at links [W1](#) and [W2](#).
11. In order to check the internet and sound for your presentation, you would have to go to [the Support Link S](#).

# Links

## Address Links:

Link M: [https://online2.uk.ac.ir/c\\_icspc\\_main/](https://online2.uk.ac.ir/c_icspc_main/)

Link B: [https://online2.uk.ac.ir/c\\_icspc\\_break/](https://online2.uk.ac.ir/c_icspc_break/)

Link T1: [https://online2.uk.ac.ir/c\\_icspc\\_talk1/](https://online2.uk.ac.ir/c_icspc_talk1/)

Link T2: [https://online2.uk.ac.ir/c\\_icspc\\_talk2/](https://online2.uk.ac.ir/c_icspc_talk2/)

Link P1: [https://online2.uk.ac.ir/c\\_icspc\\_present1/](https://online2.uk.ac.ir/c_icspc_present1/)

Link P2: [https://online2.uk.ac.ir/c\\_icspc\\_present2/](https://online2.uk.ac.ir/c_icspc_present2/)

Link W1: [https://online2.uk.ac.ir/c\\_icspc\\_workshop1/](https://online2.uk.ac.ir/c_icspc_workshop1/)

Link W2: [https://online2.uk.ac.ir/c\\_icspc\\_workshop2/](https://online2.uk.ac.ir/c_icspc_workshop2/)

Link S: [https://online2.uk.ac.ir/c\\_icspc\\_support/](https://online2.uk.ac.ir/c_icspc_support/)

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# Opening and Closing

# Opening and Closing

## Day1:12-Jan 2022

Time	Title	Link
8:15 –10:30 (AM)	Opening Ceremony	M

Link M: [https://online2.uk.ac.ir/c\\_icspc\\_main/](https://online2.uk.ac.ir/c_icspc_main/)

## Day2: 13-Jan 2022

Time	Title	Link
7:00–8:00 (PM)	Closing Ceremony	M

Link M: [https://online2.uk.ac.ir/c\\_icspc\\_main/](https://online2.uk.ac.ir/c_icspc_main/)

# Conference Program



# Conference Program

Day1: 12-Jan 2022

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Time	Title
8:15 AM-10:30 AM	Opening Ceremony
10:30 AM-11:00 AM	Break
11:00 AM-12:00 PM	Invited Talk
12:00 PM - 2:00 PM	Lunch Break
2:00 PM - 3:00 PM	Invited Talk
3:05 PM - 4:15 PM	Parallel Lectures
4:15 PM - 4:30 PM	Break
4:30 PM - 7:00 PM	Parallel Lectures
7:10 PM – 8:00 PM	Invited Talk

# Conference Program

Day2: 13-Jan 2022

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Time	Title
8:00 AM-9:00AM	Invited Talk
9:05 AM-10:15 AM	Parallel Lectures
10:15 AM-10:30 AM	Break
10:30 AM-12:30 PM	Parallel Lectures
12:30 PM-1:10 PM	Lunch Break
1:10 PM- 2:40 PM	Workshop 1
2:45 PM-4:15 PM	Workshop 2
4:15 PM-4:30 PM	Break
4:30 PM-5:30 PM	Invited Talk
5:35 PM-6:45 PM	Parallel Lectures
6:45 PM-7:00 PM	Break
7:00 PM-8:00 PM	Closing Ceremony

**Break**

# Break

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## Day1-12-Jan 2022

Time	Subject	link
10:30-11:00 (AM)	Chat and Networking	B
4:15- 4:30 (PM)	Chat and Networking	B

Link B: [https://online2.uk.ac.ir/c\\_icspc\\_break/](https://online2.uk.ac.ir/c_icspc_break/)

## Day2-13-Jan 2022

Time	Subject	link
10:15 -10:30 (AM)	Chat and Networking	B
4:15 - 4:30 (PM)	Chat and Networking	B

Link B: [https://online2.uk.ac.ir/c\\_icspc\\_break/](https://online2.uk.ac.ir/c_icspc_break/)

# Invited Talks

# Invited Talks

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## Day1: 12-Jan 2022

Time	Speaker	Title	Link
11:00(AM)-12:00(PM)	Dr. Beheshteh Sohrabi	Surface Engineering of Graphene and Its Derivatives for Various Applications	T1
2:00-3:00 (PM)	Dr. Mohammad Hossein Keshavarz	The University and Industry Relationship	T2
7:10-8:10 (PM)	Dr. Gunnar Nyman	Chemical Kinetics and Tunnelling on Interstellar Dust Grains	T1

Link T1: [https://online2.uk.ac.ir/c\\_icspc\\_talk1/](https://online2.uk.ac.ir/c_icspc_talk1/)

Link T2: [https://online2.uk.ac.ir/c\\_icspc\\_talk2/](https://online2.uk.ac.ir/c_icspc_talk2/)

## Day2: 13-Jan 2022

Time	Speaker	Title	Link
8:00–9:00 (AM)	Dr. Shahab Derakhshan	Heavy Element Transition Metal Oxides; Geometric Magnetic Frustration vs. Low Dimensional Magnetism	T1
4:30–5:30 (PM)	Dr. Aminreza Zolghadr	TiO <sub>2</sub> Nanotubes: Simulation, Synthesis, and Application	T2

Link T1: [https://online2.uk.ac.ir/c\\_icspc\\_talk1/](https://online2.uk.ac.ir/c_icspc_talk1/)

Link T2: [https://online2.uk.ac.ir/c\\_icspc\\_talk2/](https://online2.uk.ac.ir/c_icspc_talk2/)

# Parallel Lectures

## Day 1

## Day1: 12-Jan 2022

Time	Subject	Author(s)	Title	Link
3:05 PM - 3:25 PM	Theoretical	Maryam A. Rafiei, Ali Maghari	Oxygen permeation through graphdiyne membrane	<b>P1</b>
3:30 PM - 3:50 PM	Theoretical	Mojtaba Alipour, Niloofar Karimi	Photophysical properties of thermally activated delayed fluorescence emitters from the perspective of single-hybrid and double-hybrid density functional theory	<b>P1</b>
3:55 PM - 4:15 PM	Theoretical	Kobra Taji, Fatemeh Moosavi	Removal of Carbon Dioxide by Phosphonium-Based Amino Acid Ionic Liquids: Molecular Dynamics Simulation	<b>P1</b>
4:30 PM - 4:50 PM	Theoretical	Masumeh Foroutan, Borhan Mostafavi Bavani	Anisotropic wetting characteristics of water droplet on phosphorene: A molecular dynamics simulation approach	<b>P1</b>
4:55 PM - 5:15 PM	Theoretical	Faezeh Taravat, Seifollah Jalili	A new Carbon allotrope: 2D Twin Graphene	<b>P1</b>

Link P1: [https://online2.uk.ac.ir/c\\_icspc\\_present1/](https://online2.uk.ac.ir/c_icspc_present1/)

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## Day1: 12-Jan 2022

Time	Subject	Author(s)	Title	Link
5:20 PM - 5:40 PM	Theoretical	Fatemeh Nazari, Nina Alizadeh	Inclusion complexes between $\beta$ -cyclodextrin as a nanocarrier with thymol: Molecular modeling studies	<b>P1</b>
5:45 PM - 6:05 PM	Theoretical	Elahe Khosravi-Mashizi, Maryam Dehestani, Elahe Mirzaie-Khaliabadi	Conical Intersection and Non-adiabatic Dynamics on Potential Energy Surfaces of H <sub>2</sub> S <sup>+</sup> ion	<b>P1</b>
6:10 PM - 6:35 PM	Theoretical	Leila Karami	Molecular features of interaction between VEGFR-2 and Linifanib and Semaxanib using a combination of computational methods	<b>P1</b>
6:40 PM - 7:00 PM	Theoretical	Rahele Masoumifard, Mohsen Oftadeh	Investigation of Transport Properties in pure SiNW and SiNW Doped with Boron	<b>P1</b>

Link P1: [https://online2.uk.ac.ir/c\\_icspc\\_present1/](https://online2.uk.ac.ir/c_icspc_present1/)

## Day1: 12-Jan 2022

Time	Subject	Author(s)	Title	Link
3:05 PM - 3:25 PM	Practical	Negin Mokhtari, Shahrbanoo Rahman Setayesh	Synthesis of solar light responsive nanocatalysts and investigation of their performance in water splitting reaction	<b>P2</b>
3:30 PM - 3:50 PM	Practical	Zahra Dourandish, Farib Garkani Nejad, Iran Sheikhshoaie, Hadi Beitollahi	Screen-printed electrode modified with graphene quantum dots for detection of acetylcholine	<b>P2</b>
3:55 PM - 4:15 PM	Practical	Beheshteh Sohrabi	The synthesis of smart nanoparticles to pH and their applications in industry and Medicine	<b>P2</b>
4:30 PM - 4:50 PM	Practical	Zohreh Rashidi Ranjbar, Mozhde Salari Nasab	The Investigation of La(III)Ions-Doping effect on band gap of BiFeO <sub>3</sub> perovskite	<b>P2</b>
4:55 PM - 5:15 PM	Practical	Rahimi Nasim, Dalouji Vali	Effect of metal (Cu-Al)-dopants on the absorption edge of ZnO films	<b>P2</b>

Link P2: [https://online2.uk.ac.ir/c\\_icspc\\_present2/](https://online2.uk.ac.ir/c_icspc_present2/)

## Day1: 12-Jan 2022

Time	Subject	Author(s)	Title	Link
5:20 PM - 5:40 PM	Practical	Rezvaneh Amrollahi	Room temperature selective (photo) catalytic oxidation of ethanol to acetaldehyde over Pt/WO <sub>3</sub>	<b>P2</b>
5:45 PM - 6:05 PM	Practical	Ali Mehrizad	Kinetics study of catalytic ozonation process using NiO-Fe <sub>2</sub> O <sub>3</sub> catalyst for treatment of food industrial effluent	<b>P2</b>
6:10 PM - 6:35 PM	Practical	Nazila Farsad Layegh, Vahid Mohammadzadeh, Iraj Ahadzadeh, Mir Ghasem Hosseini	An inexpensive glucose biosensor based on a mixed culture microbial fuel cell (MFC) for BOD monitoring applications	<b>P2</b>
6:40 PM - 7:00 PM	Practical	Masoumeh Sohrabi, Pouneh S. Pourhosseini, Samira Ansari	Poly (ester-ether-urethane) networks and their interaction with human growth hormone: Conductometry	<b>P2</b>

Link P2: [https://online2.uk.ac.ir/c\\_icspc\\_present2/](https://online2.uk.ac.ir/c_icspc_present2/)

# Parallel Lectures

## Day 2

## Day2: 13-Jan 2022

Time	Subject	Author(s)	Title	Link
9:05 AM - 9:25 AM	Theoretical	Monireh Dehkhodaei, Adel Reisi-Vanani	Computational study of the synergistic effect of N, S atoms co-doping into monolayer graphdiyne nanosheet on hydrogen adsorption and storage	<b>P1</b>
9:30 AM - 9:50 AM	Theoretical	Razieh Razavi	Molecular Docking of Tramadol-mu-opioid Receptor	<b>P1</b>
9:55 AM - 10:15 AM	Theoretical	Mojtaba Alipour, Zahra Safari	New optimally tuned range-separated hybrids for singlet fission relevant energetics	<b>P1</b>
10:30 AM - 10:50 AM	Theoretical	Zeinab Ashrafi, Hossein Nikoofard	Prediction of oxidation potential for a series of oligopyrroles in THF solvent using DFT calculations	<b>P1</b>
10:55 AM - 11:15 AM	Theoretical	Ali Esmaeili	Quantum Chemical study of the Jahn – Teller Effect on the Distortions of XO <sub>2</sub> (X = O, S, Se, Te) Systems	<b>P1</b>

Link P1: [https://online2.uk.ac.ir/c\\_icspc\\_present1/](https://online2.uk.ac.ir/c_icspc_present1/)

## Day2: 13-Jan 2022

Time	Subject	Author(s)	Title	Link
11:20 AM - 11:40AM	Theoretical	Fahimeh Mokhtari, Mohammad Kmalvand	The effect of wall structure on sound	<b>P1</b>
11:45 AM - 12:05PM	Theoretical	Sahand Nikzat, Ali Nassimi	Proposing a trajectory-based algorithm to solve the quantum-classical Liouville equation in the mapping basis	<b>P1</b>
12:10 PM - 12:30PM	Theoretical	Khadijeh Shekoohi, Mohammad Hadi Ghatee	Structural and Dynamic Properties of Cesium Metal by Molecular Dynamics Simulation	<b>P1</b>
5:35 PM – 5:55 PM	Theoretical	Maryam Hamzeh Jouneghani, Masumeh Foroutan	Effects of Water on the Formation and the Stability of Interfacial Nano-bubble: A Molecular Dynamic Simulation	<b>P1</b>
6:00 PM - 6:20 PM	Theoretical	Elham S. Tabatabaie, Maryam Daghigh Asli	Theoretical study of the CO dissociation mechanism in $[(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CO})_2(\eta^1\text{-C}_5\text{H}_5)]$	<b>P1</b>
6:25 PM – 6:45 PM	Theoretical	Reza Safari, Hamid Hadi*	Computational study of external electric field effect on the electronic properties of a simple molecular wire	<b>P1</b>

Link P1: [https://online2.uk.ac.ir/c\\_icspc\\_present1/](https://online2.uk.ac.ir/c_icspc_present1/)

## Day2: 13-Jan 2022

Time	Subject	Author(s)	Title	Link
9:05 AM - 9:25 AM	Practical	Mahsa Mirzaei, Seyed Yousef Ebrahimipour, Maryam Mohamadinejad, Tayebeh Shampour, Fatemeh Mehrabi	Synthesis of a modified mesoporous silica for the targeted delivery of Quercetin in Buffer solution (pH=5.3)	P2
9:30 AM - 9:50 AM	Practical	Solmaz Kia	Development of molecularly imprinted polymer on ferric oxide nanoparticles modified electrode as electrochemical sensor for detection of the amount of human chorionic gonadotropin (hCG)	P2
9:55 AM - 10:15 AM	Practical	Tahereh Mohammadi, Mir Ghasem Hosseini	Transition Bimetal MOF Embedded Carbon Felt as Anode Electrode for Ethanol Fuel Cell	P2
10:30 AM - 10:50 AM	Practical	Alireza Khodabakhshi, Alireza Pouyamehr	The effect of solvent evaporation time on the properties and performance of polymer membranes based on a mixture of polyvinyl chloride and polymethyl methacrylate	P2
10:55 AM - 11:15 AM	Practical	Thorn A. Dramstad, Zahra Sohrabpour, Aaron M. Massari	Molecular Structure at the Interfaces of Submonolayer Thin Films of Sexithiophene	P2

Link P2: [https://online2.uk.ac.ir/c\\_icspc\\_present2/](https://online2.uk.ac.ir/c_icspc_present2/)

## Day2: 13-Jan 2022

Time	Subject	Author(s)	Title	Link
11:20 AM - 11:40AM	Practical	Tahereh Mohammadi, Karim Asadpour-Zeynali ,Mir Reza Majidi, Mir Ghasem Hosseini	Novel electrocatalysts for Hydrazine fuel cells: enhanced power generation by optimizing Bimetallic Ni-Co nanoparticles on Nickel Foam (NF)/ reduced graphene oxide as anode and mixed metal oxides as cathode	<b>P2</b>
11:45 AM - 12:05PM	Practical	Arash Vojood	Prebiotic Synthesis of Ethylene Glycol through Formose Reaction in Methanolic Medium	<b>P2</b>
12:10 PM - 12:30PM	Practical	Vali Alizadeh*, Ahmad Jamali Moghadam	Study of tunneling electron transfer on Graphene nanoplatelet /Self assembled monolayer modified gold electrode by electrochemical techniques	<b>P2</b>

Link P2: [https://online2.uk.ac.ir/c\\_icspc\\_present2/](https://online2.uk.ac.ir/c_icspc_present2/)



## Day2: 13-Jan 2022

Time	Subject	Author(s)	Title	Link
5:35 PM – 5:55 PM	Practical	Akbar Mobaraki	Semi-industrial synthesis of magnetic Fe <sub>3</sub> O <sub>4</sub> @SiO <sub>2</sub> @Me nanopowder to visualization of latent fingerprints	<b>P2</b>
6:00 PM - 6:20 PM	Practical	Goudarzi Samir, Dalouji Vali	Effect of Cu content on structural properties of Ni-Cu @ a-C: H thin films	<b>P2</b>
6:25 PM – 6:45 PM	Chemistry Learning	Elahe Keshavarz	Implementation of analogy method to enhance students' chemistry self-regulated learning skills	<b>P2</b>

Link P2: [https://online2.uk.ac.ir/c\\_icspc\\_present2/](https://online2.uk.ac.ir/c_icspc_present2/)

# Workshop

## Day2: 13 - Jan 2022

Time	Title	Link
1:10 – 2:40 (PM)	<b>Molecular Dynamic Simulation, Principles and Applications by Dr.Ali Mohebi</b>	W1
2:45 – 4:15 (PM)	<b>Natural Bond Orbital (NBO) Analysis by Dr.Seyed Mohammad Azami</b>	W2

Link W1: [https://online2.uk.ac.ir/c\\_icspc\\_workshop1/](https://online2.uk.ac.ir/c_icspc_workshop1/)

Link W2: [https://online2.uk.ac.ir/c\\_icspc\\_workshop2/](https://online2.uk.ac.ir/c_icspc_workshop2/)