

Curriculum Vitae

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Thesis Title:The investigation of adsorption of nitramide molecule on the surface of pristine and Ni functionalized Gallium nitride nanotubes: by computational methods

B.Sc pure chemistry

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Conferences

1. Samaneh. Barani Pour Jaber. Jahanbin Sardroodi, Alireza. Rastkar Ebrahimzadeh , The study of structure and interactions of glucose-based natural deep eutectic solvents by molecular dynamics simulation, Journal of Molecular Liquids, <https://doi.org/10.1016/j.molliq.2021.115956>
2. Samaneh. Barani Pour Jaber. Jahanbin Sardroodi, Alireza. Rastkar Ebrahimzadeh, Structure and dynamics of thymol - fatty acids based deep eutectic solvent investigated by molecular dynamics simulation, Fluid Phase Equilibria, <https://doi.org/10.1016/j.fluid.2021.113241>
3. Samaneh. Barani Pour Jaber. Jahanbin Sardroodi, Alireza. Rastkar Ebrahimzadeh, Mohammad Sadegh Avestan, **Using Molecular Dynamics Simulations to**

Understand the Effect of Fatty Acids Chain Length on Structural and Dynamic Properties of Deep Eutectic Solvents Based on Choline Chloride and Fatty Acids, chemistryselect

4. Samaneh. Barani Pour, Jaber. Jahanbin Sardroodi, Alireza. Rastkar Ebrahimzadeh, Mohammad Sadegh Avestan, **Structural and Dynamic Properties of Hydrophobic Eutectic Solvents Based on Menthol and Fatty Acids: a Molecular Dynamics Simulation Study**, scientific reports
5. Samaneh. Barani Pour, Jaber. Jahanbin Sardroodi, Alireza. Rastkar Ebrahimzadeh, **Structure and dynamics of hydrophobic deep eutectic solvents composed from terpene-fatty acids investigated by molecular dynamics simulation**, Journal of Molecular Graphics and Modelling
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6. Mahdi. Rezaei-Sameti, Samaneh .Barani pour , ***NO,N2 interaction with pristine and Si-Doped of carbon Nanoplat :Nuclear quadruple resonance study.***, The 23rd Iranian Seminar of Organic Chemistry University of Kurdistan, Sanandaj, Iran 8-10 September 2015
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8. M. Rezaei-Sameti, S. Barani Pour, H. Jolodar Behbahani, S. Abdoli. ***The first principle investigation of adsorption hydrogen cyanide on the surface of Beryllium oxide nanotube.*** The third Iranian national conference on new technologies in the chemical, petrochemical and Nanotechnology. June 2016.
9. M. Rezaei-Sameti, S. Barani Pour , **The investigation of adsorption of nitramide molecule on the surface of pristine and Ni functionalized Gallium nitride nanotubes (6,0) zigzag** , help on october 19, 2017 at Allameh Tabatabai university . Tehran , Iran

at the 4th international conference on Applied Research in chemistry science and

10. M. Rezaei-Sameti, S. Barani Pour ,**The investigation of adsorption of nitramide molecule on the surface of pristine and Pt functionalized Gallium nitride nanotubes (4,4) armchair** ,help on september 13, 2017 at Tarbiat Modarres university. Tehran , Iran **4th National Conference on Advanced Research in Chemistry and Chemical Engineering**

Workshops & Sessions

- Promotional seminar of introduction to nanotechnology, Azarbaijan Shahid Madani University, Tabriz, Iran, 2017.