SRI VENKATESWARA INTERNSHIP PROGRAM FOR RESEARCH IN ACADEMICS (SRI-VIPRA)

SRI-VIPRA

Project Report of 2024: SVP-2439

"Experimental and theoretical study of functionalized nano zeolite for their catalytic applications"

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SRIVIPRA PROJECT 2024

Title : Experimental and theoretical study of functionalized nano zeolite for their catalytic applications

Name of Mentor: Dr. Pragya Gahlot **Dr. Rekha Yadav** **Name of Department: Chemistry** **Designation: Assistant Professor**	 

List of students under the SRIVIPRA Project

S.No	Photo	Name of the student	Roll number	Course	Signature
1		Diksha	1123006	B.sc. (P.) Life Sciences Semester - III	
2		Preeti	1522027	Bsc.chemistry Honours semester-v	
3		Mahak Bahuguna	1122010	B.Sc. Life Sciences , Semester V	
4		Rohan kumar	1523048	BSc.Chemistry (Hons) Semester -3	

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Signature of Mentor **Signature of Mentor**

Certificate of Originality

This is to certify that the aforementioned students from Sri Venkateswara College have participated in the summer project SVP-2439 titled "**Experimental and theoretical study of functionalized nano zeolite for their catalytic applications**".The participants have carried out the research project work under my guidance and supervision from 1st July, 2024 to 30th September 2024. The work carried out is original and carried out in an online/offline/hybrid mode.

Signature of Mentor **Signature of Mentor**

Acknowledgements

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A special thanks for SRIVIPRA team for providing the opportunity.

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1 Title

Experimental and theoretical study of functionalized nano zeolite for their catalytic applications

2. Objectives

- To prepare Cu and Zn functionalized ZSM-5 zeolite
- To study the catalytic activity of prepared zeolite for epoxide ring opening.
- The objective of this project is to develop research aptitude in the student.
- Enhancing research capabilities of the student
- Imparting necessary IT skills for research proposes
- Developing interest in this specific research field to help in choosing the appropriate field in the early phase of their professional career

3. Methodology

a) Literature survey

Framework catalyst are important in the field of petrochemical and fine chemical industries [1]. Among which zeolites plays a major role, about 5-25 % octane enhancement in petroleum refining is done on ZSM-5 only [2]. Numerous uses in the fields of catalysis, adsorption, and ion transport have been demonstrated by the customized synthesis of open framework materials with specified molecular sieve topologies. Several reports of studies on silicate-based molecular sieves and have been thoroughly investigated in several studies on catalysis.

ZSM-5 (Zeolite Socony Mobil-5) is a prominent catalyst in petrochemical industries and environmental applications, recognized for its unique structural and catalytic properties. This aluminosilicate zeolite features a three-dimensional framework composed of interconnecting channels and cavities, which allows for selective adsorption and transformation of hydrocarbons. Its structure comprises 10-membered ring openings that facilitate shape-selective catalysis, making ZSM-5 highly effective in processes such as catalytic cracking, alkylation, and the conversion of dimethyl ether to olefins [3]. The high surface area and thermal stability of ZSM-5 contribute to its exceptional catalytic activity, enabling the efficient transformation of various feedstocks into valuable products, including gasoline-range hydrocarbons.

The olefin conversion, in particular, highlights the utility of ZSM-5 in sustainable chemistry, [4]. The zeolite's acidic sites, which can be modulated through ion-exchange or dealumination, enhance its catalytic efficiency by providing optimal conditions for protonation and subsequent reactions [5]. This adaptability not only increases the yield of desired products but also minimizes the formation of by products, thus improving overall process efficiency and selectivity.

Furthermore, ZSM-5 has been studied for its role in environmental applications, such as the catalytic removal of pollutants and the conversion of waste into valuable chemicals. Its ability to catalyse the oxidative degradation of volatile organic compounds (VOCs) underscores its importance in addressing environmental concerns (oxidative decomposition of the binary mixtures of chlorinated volatile organic compounds (CVOCs) [1,2-dichloroethane (DCE), dichloromethane (DCM), and trichloroethylene(TCE)] over H-ZSM-5 zeolite). [6]. Ongoing research continues to explore the potential of modified ZSM-5 catalysts, including metal-doping and structural optimization, to enhance catalytic performance and broaden their applicability [7]. The continuous advancements in ZSM-5 technology reflect its critical role in both traditional petrochemical processes and the emerging fields of renewable energy and green chemistry.

In conclusion, ZSM-5 stands as a vital catalyst, bridging the gap between conventional hydrocarbon processing and sustainable chemical production. Its distinctive properties and versatility underscore its significance in the ongoing evolution of catalysis.

b) Preparation of Catalysts

Preparation of ZSM-5 catalysts using hydrothermal synthesis- Preparation of ZSM-5 was done as per procedure discussed by Bhat et al. For synthesis, three different solutions were prepared A1=45.697 g sodium sulfate + 56.6 g water, A2= 3.965 g TEBA + 20 g water and A3=0.662 g Al_2 $(SO_4)_3$ + 16 H_2O + 2.5 g sulfuric acid and 26 g water where TEBA: Triethyl n-butyl ammonium bromide.
Solutions A2 and A3 were added to A1 drop by drop with stirring. After the complete addition the gel was stirred for 2 h and its pH was adjusted to 10.5 by adding dropwise dilute sulfuric acid.
The as-synthesized zeolite samples are washed with distilled water and dried. The dried material was calcined in air [8].
Cu-ZSM-5- 1% Copper sulfate solutions was prepared in ethanol and were impregnated on 1 g calcined ZSM-5. The catalyst was then calcined again [6].

Characterization- The as-synthesized zeolite samples were characterized for structural, morphological, and acidity features by physicochemical techniques such as XRD, SEM, and TPD of ammonia. The Si/Al ratio was determined by atomic absorption spectrophotometry.

c) Study of catalytic activity of the catalysts
The prepared materials were studied for epoxide ring opening at various experimental conditions.

d) Use of IT tools
Different IT tools including PPT, word, Origin etc were used.

e) Result and Discussion
The catalyst was prepared successfully and showed good conversion for epoxide ring opening.

f) References

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[7] Derouane, E. G. (2001). Catalysis in the 21st Century, Lessons from the Past, Challenges for the Future. *Cattech*, *5*, 214-225.
[8] Bhat, Y. S., Das, J., Rao, K. V., & Halgeri, A. B. (1996). Inactivation of external surface of ZSM-5: zeolite morphology, crystal size, and catalytic activity. *Journal of catalysis*, *159*(2), 368-374.

4. Learning outcomes

The students can

- Search on Academic Search Engines and filter the relevant literature
- Use Text Management Tools to write and improvise the literature
- Study the catalytic applications

5. Future prospects

- Preparation of Zn, Fe and Co functionalized ZSM-5 catalysts
- Study the catalytic activities of the catalyst prepared.
- Extending the same approach to other zeolite systems.