Ph.D. Viva-Voce Examination

The Ph.D. viva-voce examination of Mr. Sonit Balyan (2014CHZ8178) will be held on July 23rd, 2021 at 9.30 AM. The title of his thesis is "Understanding Catalysis by Molybdenum Carbide Nanoclusters in Mo/HZSM-5 Catalyst for Methane Dehydroaromatization". The examination will be conducted through video conferencing for which the link will be shared separately.

All are cordially invited to attend the seminar. The abstract of the seminar is attached herewith.

Date and Time: July 23rd, 2021 (Friday) at 9.30 AM.

Through video conferencing.

Copy to:
1. Prof. Sanjay M. Mahajani (Department of Chemical Engineering, IIT Bombay),
2. Dean (Academics), IIT Delhi
3. Associate Dean, Academics (PGS&R), IIT Delhi
4. HOD/DRC Chair, Department of Chemical Engineering
5. SRC Members: Prof. Rajesh Khanna, Prof. Sreeedevi Upadhyayula, and Prof. Ravi P. Singh (Chemistry Dept.)
6. All Faculty members, Department of Chemical Engineering
7. DRC Secretary/Ph.D. Coordinator and Secretary, Department of Chemical Engineering
8. Dy. Registrar (Accounts)
9. All ChE faculty and Students
10. Department Notice Board- Ph.D./M.Tech Students

Abstract Overleaf:
Understanding Catalysis by Molybdenum Carbide Nanoclusters in Mo/HZSM-5 Catalyst for Methane Dehydroaromatization

Abstract
Single step methane conversion to value added product is an economical route to exploit natural gas reservoirs from industrial perspective. A bifunctional catalyst having active molybdenum species supported on zeolite (Mo/HZSM-5) is well-studied for high aromatic selectivity in methane dehydroaromatization (MDA) process. However, the catalyst is known to deactivate due to carbon deposition over time-on-stream. The stabilization of active molybdenum carbide (Mo$_2$C$_6$) species anchored on the inner side of the zeolite framework can reduce carbon deposition. For this purpose, a massively parallel cascade genetic algorithm (cGA) search is employed to scan the potential energy surface for determining all possible low-energy structures of active Mo$_2$C$_6$ species. This search is further combined with density functional theory (DFT) calculations to study catalytic activity of the most stable and metastable Mo$_2$C$_6$ clusters for C-H bond activation and C-C coupling reactions to form ethylene and acetylene in MDA process. Theoretical findings on the evolution and anchoring of active Mo$_2$C$_6$ species on HZSM-5 provides a rational for implementing desirable experimental conditions to improve the stability of the active species. This is achieved by obtaining a higher amount of Mo carbide by tailoring the carburizing agent. A strategy to stabilize these primary molybdenum oxide/carbide species over the zeolite after subsequent thermal and chemical treatment is proposed. It is achieved by thermal treatment of molybdenum precursors and conversion of orthorhombic α-MoO$_3$ to metastable hexagonal h-MoO$_3$ via hydrothermal topotactic transformation. In this work, the role of Mo precursor interaction with the zeolite in altering catalyst reactivity is studied. In order to achieve higher aromatic (benzene) selectivity the Brønsted acidity of HZSM-5 zeolite is moderated by pretreating it with boric acid. Moreover, this novel strategy of controlling the Brønsted acidity of HZSM-5 zeolite enhances catalyst stability in MDA by reducing the agglomeration of active Mo$_2$C$_6$ species and the carbon deposition. Overall the dissertation provides a molecular level insights of active catalyst site of the reaction. In turn, this study provides a guiding tool for rational catalyst design by specifying the choice of Mo precursor, carburizing condition and zeolite treatment for MDA process.