1. Abstract Title: A Review of Representative Periodic DFT Model on Structure and Properties of Chromia-silica Catalyst in Ethylene Polymerization

2. All Authors: Sahar Bayat, M.S. Catalysis Chemistry, Abadgaran Construction Chemicals Manufacturer. Seyyed Alborz Majzoob Hosseini, M.S. Chemical Engineering, Abadgaran Construction Chemicals Manufacturer.


4. Short Description of what will be discussed during the presentation:

As an important type of plastic, polyethylene (PE) is a most commonly used in various fields such as containers, constructions, automobile parts, packing films, and pipe materials. Chromium-based catalyst systems, including SiO$_2$-supported inorganic chromium oxide catalyst (Phillips catalyst) and SiO$_2$-supported organic silyl chromate catalyst, are widely used as important industrial catalysts to manufacture polyethylene products, main of them is high-density polyethylene (HDPE). The silica support plays an important role in directing the morphology of the polymer particles. The neglect of the silica surface may introduce some artificial effects and provides unrealistic environment for the adsorption of monomer on the active chromium center. Nowadays, with the improvement of computing resources and the development of quantum methodologies, full quantum calculations using a large surface-supported model or a periodic model of silica gel surface can be performed. Computational modelling, taking advantage of growing computer power, enables for development of advanced models representing surface metal
species. Density functional theory (DFT) methods, offering a good balance between the accuracy and the cost, are nowadays commonly used in the field of computational catalysis. Theoretical investigations are helpful in interpretation of spectroscopic data concerning supported transition metal oxide species. Quantum chemistry methods, especially when combined with advanced models of the surface, can also provide complementary information about the catalytic system, not accessible at this moment by experimental techniques.

In this paper, we primarily focus on transition-metal catalyzed reactions involved in heterogeneous olefins (α-olefins) polymerization and review recent studies that benefit from ab initio techniques including cluster and periodic modelings. First, we briefly give an explanation of current explorations in the computational modelings which are extensively used in transition-metal reaction studies. Further, we review specifically recent innovations in chromia-silica supported heterogeneous ethylene polymerization computational methodologies.

5. What will the audience take away from your presentation?
- They will know the fundamentals of using statistics and databases to integrate chemical theories and modeling with experimental observations.
- Interpretation and prediction of complex system behavior at an atomic scale opens avenue for further innovations in chemistry and materials science.
- Specifically, DFT computational methods could be applied in synthesis-related systems and processing parameters.
- The recent studies demonstrated in this work lay a solid foundation for further improvement of high-grade bimodal HDPE pipe materials.

6. Is this abstract connected to an organized session? If yes, please provide full session title.

No.

7. Biography of presenting author
Sahar Bayat

Sahar Bayat is an R&D member at Abadgaran Construction Chemicals Manufacturer, where she researches with the aim of developing materials quality while persuading an in-depth prospective to customers’ willing and environment preservation. She graduated from Shahid Beheshti University, with bachelor's degree in applied chemistry, and where she is currently doing her master research in theoretical ab-initio studies in heterogeneous catalysis under the supervision of Dr. S. Shahab Naghavi. Beside working on catalysis reactions and computational chemistry, her research focuses on olefins(α-olefins) thermal and redox polymerization for further detection of characterized polymers which enhance flowability and durability of cementitious particles.

Author Details:

Full Name: Sahar Bayat
Contact Number: 00989122681493
Country: Iran
Category: Poster Presentation
Session Name: Computational Catalysis
Email: Sahariii_bayat@yahoo.com (and or sa.bayat@mail.sbu.ac.ir)