# Innovative Applications of Mo(W)-Based Catalysts in the Petroleum and Chemical Industry: Emerging Research and Opportunities

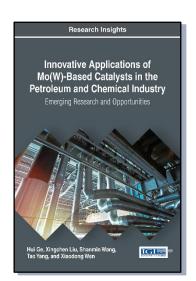
Part of the Advances in Chemical and Materials Engineering Book Series

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## **Description:**

Mo(W)-Based Catalysts have the capacity to drastically impact many different industries. Research on their most current applications is important for the success of many organizations and companies, specifically the chemical and petroleum industries.

Innovative Applications of Mo(W)-Based Catalysts in the Petroleum and Chemical Industry: Emerging Research and Opportunities is an informative resource that overviews emerging methods and techniques that incorporate 2D layer Mo(W) dichalcogenides. Featuring extensive coverage on a range of subjects including 2D nanosheets, hybridization, dichacogenides, and oxide based catalysts, this is an ideal publication for academicians, students, engineers, and researchers seeking insight on the latest advancements in Mo(W)-Based catalyst applications.



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# **Topics Covered:**

- 2D Nanosheets
- 3D Nano-Catalysts
- Boride
- CVD Method
- Dichalcogenides
- Nanosheets
- Nitride
- Oxide Based Catalysts
- Phosphide
- Wet Chemical Method

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3D catalysts of Mo(W) carbide, nitride, oxide, phosphide and boride

Chapter 4

Low-dimensional molybdenum-based catalytic materials from theoretical perspectives

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Summary and Perspectives

**Hui Ge received his Ph.D.** degree from Institute of Coal Chemistry, Chinese Academy of Sciences in 2009 and then worked there as an associate professor. He has been researching on synthesis, characterization, and catalytic application of Mo based materials and nanostructured composites. And He has developed series of CoMo and NiMo catalysts for hydrodesulfurization of gasoline and diesel. He has rich experience in synthesis of novel catalytic material and DFT calculation of the structure, properties and reaction mechanism of transit metal catalyst. His scientific interests include heterogeneous catalysis, 2D materials, theory calculation, new energy and environmental science.

Xingchen Liu is a research scientist at the Institute of Coal Chemistry, Chinese Academy of Sciences, China. He was born in 1984 in Shanxi Province, China. In 2002, he left for college education at Jilin University, where he got the degree of Bachelor of Science majored in chemistry in 2006, and the degree of Master of Science majored in physical chemistry in 2009. Afterwards, he studied in the field of theoretical chemistry under the supervision of Prof. Dennis Salahub at the University of Calgary as a graduate student. In 2015, after the Ph.D. graduation, he joined Dr. Xiaodong Wen's lab at the Institute of Coal Chemistry, Chinese Academy of Sciences and worked as a research scientist since then. Xingchen Liu's research focuses on the theoretical modelling of the heterogeneous catalytic materials at extreme conditions and complex environments. He also works on method developments for searching of reactions paths.

Shanmin Wang is a high-pressure (P) physicist and material scientist with extensive experience in diffraction studies of crystal structures, equations of state, phase transitions, and strongly correlated 3d systems, and hard/superhard ceramics. He has been working on synthesis, characterization, and modeling of catalyst materials, semiconductors and superconductors, hard/superhard materials, and nanostructured composites at high pressures. Prof. Wang has rich experience in use of high-P large-volume press and diamond-anvil cell. Very recently, using newly formulated high-P reaction routes, he has recently synthesized a number of novel transition-metal nitrides, including W2N3, W3N4, and 3R–MoN2, and most of them are potential industrial catalysts possessing superior catalytic properties. Overall, his scientific interests include new energy researches, condensed matter physics, materials sciences, and crystallography. His technical specialties cover high P-T and high-P/low-T instrumentations for neutron and synchrotron x-ray diffraction.

**Tao Yang** received her Master degree from Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences in 2005. In 2008, Dr. Tao Yang got her Ph.D. degree from Institute of Coal Chemistry, Chinese Academy of Sciences, and worked on Water-Gas-Shift reaction mechanism on iron oxides. After graduating, Dr. Tao Yang joined the group of Prof. Roald Hoffmann (the 1981 Nobel Prize in Chemistry) in Cornell University as a research scholar. In 2015, Dr. Tao Yang joined the group of Prof. Baojian Shen in State Key Laboratory of Heavy Oil Processing, China University of Petroleum as a research scientist, and is working on iron-based catalysts for hydrodesulfurization via theoretical approaches, including DFT and MD. Dr. Tao Yang's interests is to pursue and hunt a "route" to rational design Fe-based materials and catalysts with desired functionality.

Xiaodong Wen received his Ph.D. degree from Chinese Academy of Sciences in 2007. After his Ph.D., Prof. Wen joined the group of Prof. Roald Hoffmann (the 1981 Nobel Prize in Chemistry) and Dr. Neil Ashcroft at Cornell University as a postdoc. After three years, in 2010, he joined the group T-1 in LANL as a Seaborg Institute fellow, and worked on predicting actinide/magnetic materials using theoretical tools, and developing strongly correlated method. From 2014, Prof. Xiaodong Wen was selected as Hundred People Plan Program in Chinese Academy of Sciences, and awarded as National Thousand Young Talents Program of China. The researches of Prof. Wen are focused on rational design of catalysts (especially for carbon-based energy conversion) and materials (sustainable energy related materials) combining experimental and theoretical approach.