

1. Record Nr.	UNINA9910254027003321
Titolo	Structure and Modeling of Complex Petroleum Mixtures // edited by Chunming Xu, Quan Shi
Pubbl/distr/stampa	Cham : , : Springer International Publishing : , : Imprint : Springer, , 2016
ISBN	3-319-32321-0
Edizione	[1st ed. 2016.]
Descrizione fisica	1 online resource (VII, 182 p.)
Collana	Structure and Bonding, , 0081-5993 ; ; 168
Disciplina	665.5
Soggetti	Chemistry, Physical and theoretical Chemical engineering Fossil fuels Physical Chemistry Theoretical and Computational Chemistry Industrial Chemistry/Chemical Engineering Fossil Fuels (incl. Carbon Capture)
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Intro -- Aims and Scope -- Preface -- Contents -- Molecular Structure and Association Behavior of Petroleum Asphaltene -- 1 Introduction -- 2 Chemical Structure of Asphaltene Molecule -- 2.1 Molecular Weight (MW) -- 2.2 Detail Composition and Structure -- 3 Molecular Interactions and Aggregation Models -- 3.1 Asphaltene Molecular Interactions -- 3.1.1 Acid-Base Interactions -- 3.1.2 Hydrogen Bonding -- 3.1.3 Coordination -- 3.1.4 pi-pi Stacking -- 3.2 Structural Model of Asphaltene Aggregation -- 3.2.1 Yen Model -- 3.2.2 Yen-Mullins Model -- 3.2.3 Gray's Model -- 3.2.4 Yarranton's Model -- 3.2.5 PAC Model -- 4 Asphaltene Deposition -- 4.1 Asphaltene Micellization and Aggregation -- 4.2 Asphaltene Nanoaggregation -- 4.3 Clustering of Asphaltene Nanoaggregates -- 5 Size Distribution of Asphaltene Monomers and Aggregates -- 5.1 Size of Asphaltene Monomers -- 5.2 Size of Asphaltene Aggregates -- 5.3 Effects on Size of Asphaltenes -- 6 Molecular Simulation -- 6.1 Atomic Level -- 6.2 Coarse-Grained Level -- 7 Thermodynamic Models and Oil Compatibility -- 8

Concluding Remarks -- References -- Porphyrins in Heavy Petroleums: A Review -- 1 Introduction -- 2 Vanadium and Nickel Compounds in Heavy Petroleums -- 3 Isolation of Porphyrins from Heavy Petroleums -- 3.1 Solvent Extraction for Primary Enrichment Separation -- 3.2 Column Chromatography for Porphyrins Separation -- 3.3 Purification Methods for the Specific Porphyrins -- 4 Chemical Characterization of Porphyrins -- 4.1 Identification and Quantification by UV-Visible Spectroscopy -- 4.2 Molecular Characterization by Mass Spectrometry -- 4.3 Structure Characterization by X-Ray Absorption Spectroscopy -- 4.4 Other Methods -- 5 Porphyrins as a Maturity Parameter for Petroleum Thermal Evolution -- 6 Demetallization Technologies for Petroleum Upgrading -- 7 Summary and Future Prospects -- References.

Ruthenium Ion-Catalyzed Oxidation for Petroleum Molecule Structural Features: A Review -- 1 Introduction -- 2 Principles and Methodology -- 2.1 Mechanism of RICO Catalytic Reaction -- 2.2 Basic Reactions of RICO -- 2.3 Other Side Reactions Occurring in RICO System -- 2.4 Quantitative Analysis of RICO Products -- 3 RICO Revealed Molecular Structure of Heavy Petroleum Fractions -- 3.1 Asphaltenes -- 3.2 Other Heavy Petroleum Fractions -- 3.3 Carbon Residue on Catalyst -- 3.4 Kerogen -- 4 Summary and Future Prospects -- References --

Molecular-Level Composition and Reaction Modeling for Heavy Petroleum Complex System -- 1 Introduction -- 2 Composition Model for Heavy Oil -- 2.1 Qualitative Molecular Information Determination -- 2.1.1 Core Representation -- 2.1.2 SC and IL Representation -- 2.1.3 Resid Molecule Sampling -- 2.2 Quantitative Molecular Information Determination -- 2.2.1 Quantitative Sampling Protocol -- 2.2.2 Model Optimization and Representative Results -- 3 Reaction Model for Heavy Oil -- 3.1 ARM Reaction Network Analysis -- 3.2 ARM Model Equation -- 3.3 Kinetic Parameters: LFER -- 3.4 Post-reaction Sampling and Product Property Estimation -- 3.5 Representative Results of a Resid Pyrolysis Model -- 4 Summary -- References -- Molecular Modeling for Petroleum-Related Applications -- 1 Introduction -- 2 Theory and Methods -- 2.1 Classification -- 2.2 QM-Based Methods -- 2.2.1 Ab Initio Methods -- 2.2.2 Semiempirical Methods -- 2.2.3 DFT -- 2.3 Force-Field-Based Methods -- 2.4 MM Models -- 2.5 MC Methods -- 2.6 MD Methods -- 3 Applications in Heavy Oil Chemistry -- 3.1 Improved B-L Method -- 3.2 Most Probable Molecular Conformation of Heavy Oil -- 4 Applications in Catalyst Development -- 4.1 Adsorption -- 4.1.1 Adsorption Isotherms -- 4.1.2 Adsorption Thermodynamics -- 4.1.3 Adsorption Sites -- 4.2 Diffusion -- 4.2.1 Diffusion in Zeolites. 4.2.2 Zeolite Modification -- 4.2.3 Diffusion in Hierarchical Zeolite -- 4.3 Catalyst Structure -- 5 Applications in Reactions of Refining Processes -- 5.1 Desulfurization -- 5.1.1 Hydrodesulfurization (HDS) -- 5.1.2 RADS -- 5.2 Hydrodenitrogenation (HDN) -- 5.3 Alkylation -- 5.4 Isomerization -- 5.5 Hydrodeoxygenation (HDO) -- 6 Summary and Prospects -- References -- Index.

---

## Sommario/riassunto

Chemical structure and bonding. The scope of the series spans the entire Periodic Table and addresses structure and bonding issues associated with all of the elements. It also focuses attention on new and developing areas of modern structural and theoretical chemistry such as nanostructures, molecular electronics, designed molecular solids, surfaces, metal clusters and supramolecular structures. Physical and spectroscopic techniques used to determine, examine and model structures fall within the purview of Structure and Bonding to the extent that the focus is on the scientific results obtained and not on specialist information concerning the techniques themselves. Issues associated with the development of bonding models and generalizations that

illuminate the reactivity pathways and rates of chemical processes are also relevant. The individual volumes in the series are thematic. The goal of each volume is to give the reader, whether at a university or in industry, a comprehensive overview of an area where new insights are emerging that are of interest to a larger scientific audience.

---