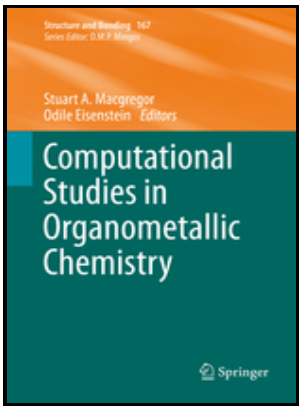
Computational organometallic chemistry

Marcel Dekker - Computational Organometallic Chemistry with Force Fields



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Interplay between Theory and Experiment: Computational Organometallic and Transition Metal Chemistry

Theoretical Study on the Mechanism of Ni-Catalyzed Alkyl-Alkyl Suzuki Cross-Coupling. ACS Catalysis 2020, 10 13 , 7136-7145. Topics addressed include: DFT studies on zirconium-mediated reactions, force field methods in organometallic chemistry, hydrogenation of π-systems, oxidative functionalization of unactivated C-H bonds and olefins, the osmylation reaction, and cobalt carbonyl clusters.

Interplay between Theory and Experiment: Computational Organometallic and Transition Metal Chemistry

We begin by examining the use of computational chemistry to elucidate the details of some unusual chemical bonds.

Computational (DFT) Studies of Organometallic Complexes (Chemistry & Computer Science)

Matching experimental results with computational methods often leads to greater understanding of fundamental chemical properties and reactivity patterns of such complexes. Organometallics 2013, 32 3 , 752-761.

Interplay between Theory and Experiment: Computational Organometallic and Transition Metal Chemistry

Organometallics 2014, 33 5 , 1126-1134. Inorganic Chemistry 2017, 56 24 , 14888-14899. Masoud Nabavizadeh, Fatemeh Niroomand Hosseini, Fatemeh Niknam, Peyman Hamidizadeh, S.

Computational (DFT) Studies of Organometallic Complexes (Chemistry & Computer Science)

Jafar Hoseini, Fatemeh Raoof, Mahdi M. Reactions of osmapyridinium with terminal alkynes. This snapshot of state-of-the-art computational studies provides an overview of the vast field of computational organometallic chemistry.

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WHAT SHOULD I DO NEXT? MacKerell JAD, Bashford D, Bellott M, Dunbrack JRL, Evanseck JD, Field MJ, Fischer S, Gao J, Guo H, Ha S, Joseph-McCarthy D, Kuchnir L, Kuczera K, Lau FTK, Mattos C, Michnick S, Ngo T, Nguyen DT, Prodhom B, Reiher I, Roux B,

Schlenkrich M, Smith JC, Stote R, Straub J, Watanabe M, Wiorkiewicz-Kuczera J, Yin D, Karplus M 1998 All atom empirical potential for molecular modeling and dynamics studies of proteins. We then give an example of how theoretical calculations aided the structural determination of a Î° 2- N, N chelate ruthenium complex formed upon heating an intermediate benzonitrile-coordinated complex.

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