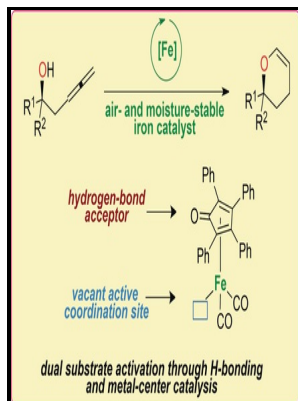


Computational organometallic chemistry

Marcel Dekker - Interplay between Theory and Experiment: Computational Organometallic and Transition Metal Chemistry



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- Organometallic chemistry
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Computational tools for mechanistic discrimination in the reductive and metathesis coupling reactions mediated by titanium IV isopropoxide.

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Two particular applications of VALBOND-TRANS to an Ir III and a Pt II complex are presented. Journal of Chemical Theory and Computation 2018, 14 7 , 3428-3439.

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Together, they illustrate some of the achievements that are possible with a fruitful union of experiment and theory. ACS Catalysis 2015, 5 11 , 6640-6647. In each case, theoretical calculations provide particular insight into the electronic structure of the chemical bonds.

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Organometallics 2013, 32 3 , 752-761.

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

Reactions of osmapyridinium with terminal alkynes. Masoud Nabavizadeh, Fatemeh Niroomand Hosseini, Fatemeh Niknam, Peyman Hamidzadeh, S.

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Mechanistic insight into cobalt-catalyzed stereodivergent semihydrogenation of alkynes: The story of selectivity control. Organometallics 2017, 36 23 , 4611-4619. Computational Studies of Synthetically Relevant Homogeneous Organometallic Catalysis Involving Ni, Pd, Ir, and Rh: An

Overview of Commonly Employed DFT Methods and Mechanistic Insights.

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