Record Nr. UNINA9910254025803321 Computational Studies in Organometallic Chemistry / / edited by Stuart Titolo A. Macgregor, Odile Eisenstein Cham:,: Springer International Publishing:,: Imprint: Springer,, Pubbl/distr/stampa 2016 **ISBN** 3-319-31638-9 Edizione [1st ed. 2016.] 1 online resource (VII, 181 p.) Descrizione fisica Collana Structure and Bonding, , 0081-5993; ; 167 Disciplina 547.05 Soggetti Organometallic chemistry Chemistry, Physical and theoretical Inorganic chemistry Organometallic Chemistry Theoretical and Computational Chemistry Inorganic Chemistry Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Note generali Includes index. Nota di contenuto D10-ML2 Complexes: Structure, Bonding and Catalytic Activity --Computation of Excited States of Transition Metal Complexes --Reactivities and Electronic Properties of Boryl Ligands -- QM/MM studies in Organometallic Chemistry -- Dynamic Studies in Organometallic Chemistry -- CH activation, from transition metal to main group systems -- Computation and experiment into alignment in Organometallic Chemistry: Are we there. The series Structure and Bonding publishes critical Reviews on Topics Sommario/riassunto of Research concerned with 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. Thus each review within the volume critically surveys one aspect of that topic and places it within the context of the volume as a whole. The most significant developments of the last 5 to 10 years should be presented using selected examples to illustrate the principles discussed. A description of the physical basis of the experimental techniques that have been used to provide the primary data may also be appropriate, if it has not been covered in detail elsewhere. The coverage need not be exhaustive in data, but should rather be conceptual, concentrating on the new principles being developed that will allow the reader, who is not a specialist in the area covered, to understand the data presented. Discussion of possible future research directions in the area is welcomed.