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Nota di contenuto	General introduction -- Computational methods -- Objectives -- The Negishi reaction mechanism -- The Cu-free Sonogashira reaction mechanism -- An asymmetric Suzuki-Miyaura reaction mechanism -- General conclusions.
Sommario/riassunto	Find out how theoretical calculations are used to determine, elucidate and propose mechanisms for Pd-catalyzed C-C cross-coupling reactions in Max Garcia Melchor's outstanding thesis. Garcia Melchor investigates one of the most significant and useful types of reactions in modern organic synthesis; the Pd-cross coupling reaction. Due to its versatility, broad scope and selectivity under mild conditions, this type of reaction can now be applied in fields as diverse as the agrochemical and pharmaceutical industry. Garcia Melchor studies the reaction intermediates and transition states involved in the Negishi, the copper-free Sonogashira and the asymmetric version of Suzuki-Miyaura coupling. He also characterizes and provides a detailed picture of the associated reaction mechanisms. The author has won numerous prizes for this work which has led to over eight publications in internationally renowned journals.