Modelling Kinetics and Thermodynamics of Catalytic Metal-Organic Cages

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Gregori Ujaque received his Ph.D. from the UAB in 1999 working on the application of theoretical methods to transition metal chemistry (with A. Lledós and F. Maseras). Then, he spent two years as a postdoc at UCLA working on rational design of catalytic antibodies and organic reactions by computer simulations (with Ken Houk). He returned to the UAB with a "Ramon y Cajal" position, becoming lecturer in 2007. He has been working on the application of computational methods (QM and QM/MM methods, more recently AIMD and QM/MM-MD methods) to the understanding of homogeneous catalysis. Among other catalytic processes, he enjoys working on cross-coupling, hydrogenation, oxidation, gold catalyzed reactions, etc. Lately he opened a new research line devoted to supramolecular chemistry and its applications to catalysis. He served as associate editor of the journal *Anales de Química* from the RSEQ during the 2018-2020 period and he is part of the editorial board of the journal *Catalysts*. G. Ujaque is the current President of the "Societat Catalana de Química" since 2020.