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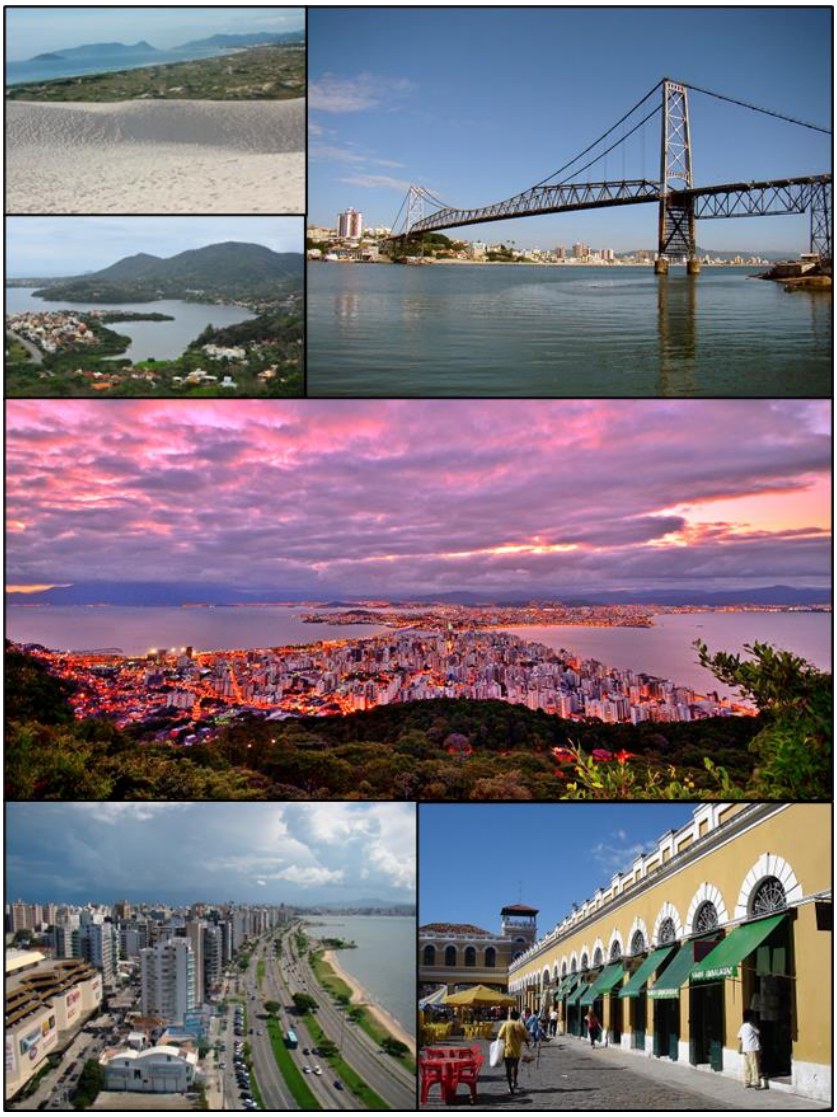
ABSTRACT BOOK



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Kinetics of Pd Cross-Coupling Reactions via Single-Molecule Fluorescence Microscopy: Higher Catalytic Efficiency from $Pd_2(0)$ dimers

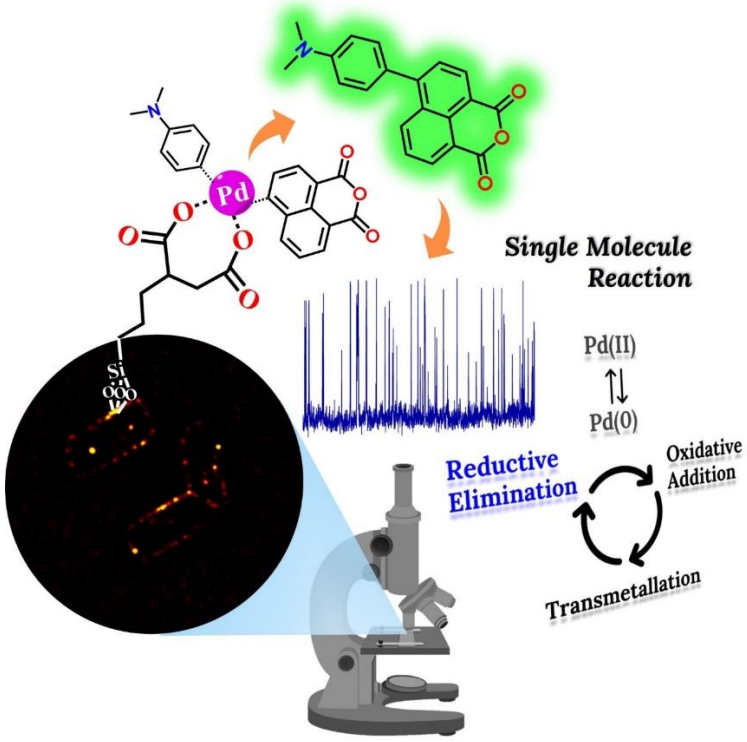
Gehlen, Marcelo Henrique*; Reis, Izadora Fonseca

*Corresponding author: marcelog@iqsc.usp.br

Institute of Chemistry of São Carlos, University of São Paulo, São Carlos, SP, Brazil

Keywords: catalyst turnover frequency (SM-TOF), fluorescence intermittency, stochastic simulation

We have introduced a statistical model of analysis of fluorescence intermittency of fluorophore formed by Pd catalyst that allows a direct determination of the single-molecule turnover frequency (SM-TOF) of the catalytic process [1]. Using extremely diluted catalyst dispersion of Pd in glass surface, Pd ligand in glass and in zeolite microparticle, SM-TOF is evaluated in four Suzuki-Miyaura cross-coupling reactions. The results obtained in our study point out that the way of loading Pd catalyst in a surface or in microparticle template defines the SM-TOF of a given cross-coupling reaction. The use of micro-zeolite template with surface bound Pd ligand is a more efficient method for achieving higher SM-TOF when compared with Pd adsorbed or complexed with surface sites well dispersed on a flat glass. The highest effectiveness in micro-zeolite template system is ascribed to a cooperativity of Pd with more than a single metal complex supported by succinic diacid ligand in close proximity as catalyst center. Stochastic simulation of the reaction cycle considering the presence of $Pd_2(0)$ dimers corroborates with the assumption of catalyst cooperativity in micro-zeolite template.



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References:

[1] Reis, I. F.; Gehlen, M. H. *J. Phys. Chem. Letters* **2024**, 2352-2358.