DFT and machine learning techniques towards the study of copper-catalyzed Suzuki-Miyaura reactions

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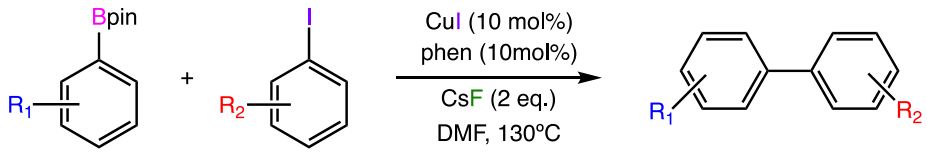
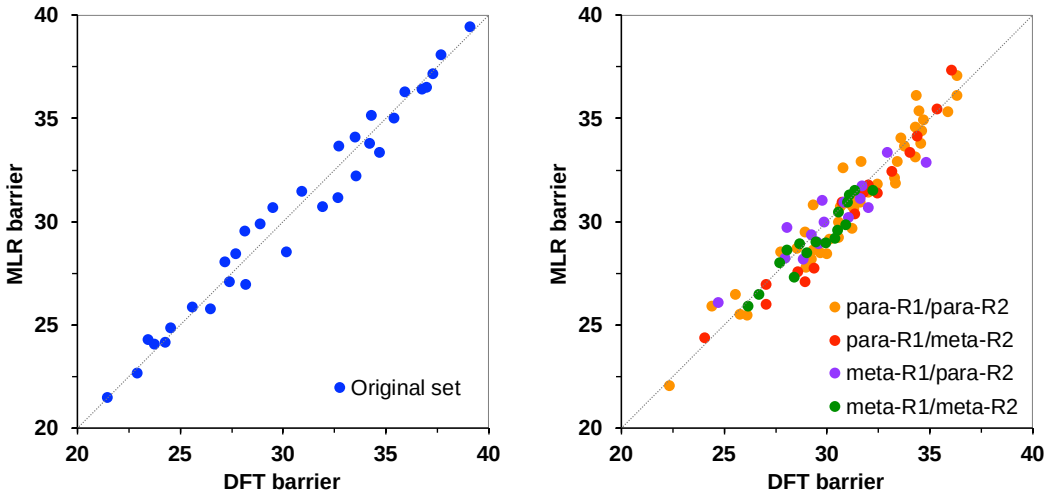
Copper catalysts can be successfully employed as a replacement in reactions employing precious metals such as Pd. A good example of this is the Cu-catalyzed Suzuki-Miyaura coupling between aryl boronate esters and aryl iodides.[1] This reaction has been computationally explored to propose a plausible mechanism that is able to explain the observed reactivity.



Once a reasonable mechanism has been determined, DFT calculations coupled with machine learning techniques have been applied to compute and predict the overall reaction barrier of reactions where the substituents on the boronate ester (R_1) and aryl iodide (R_2), placed in *para*- and *meta*-positions, cover the full range of electronic properties. In this way we can compute and predict the overall reaction barrier of any reaction of the same type by just computing the CM-5 charge of the boron atom of the boronate ester and the charge of the *ipso* carbon of the aryl iodide.



Referencias

[1] Y. P. Budiman, A. Friedrich, U. Radius, T. B. Marder, *ChemCatChem*, **2019**, *11*, 5387-5396.