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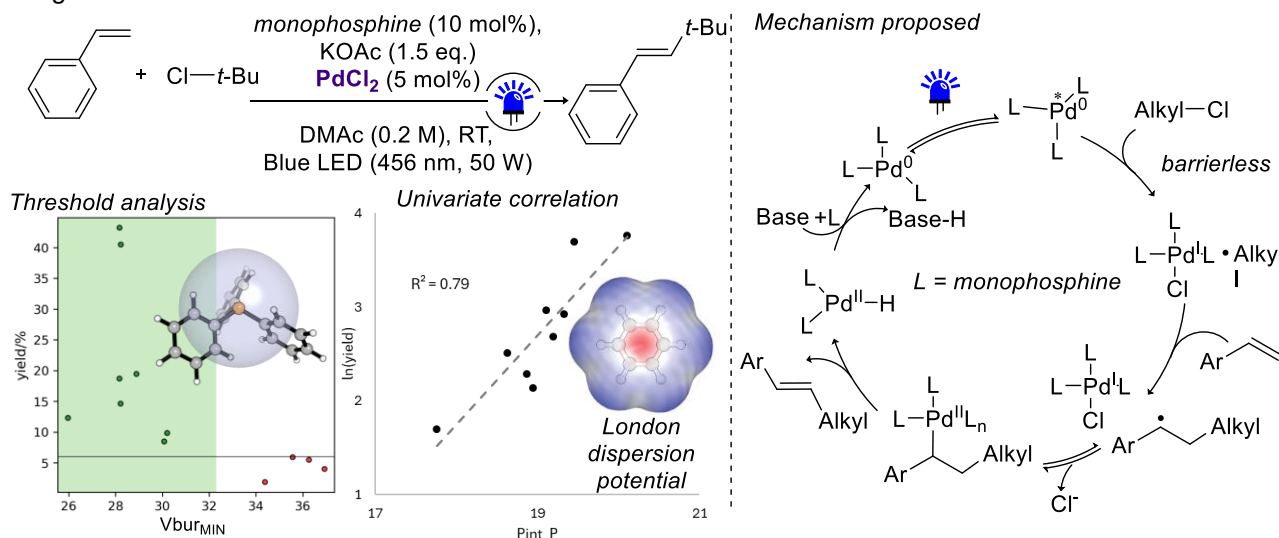
Mechanistic investigation of Pd-photocatalyzed Heck reaction

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ABSTRACT

Coupling reactions have proven to be incredibly useful in organic synthesis, both in academia and industry, and palladium as a catalyst proves to be extremely efficient and versatile, where in addition to coupling it is also capable of cascade reactions.¹ The development of these reactions via photochemical pathway allows access to reactivities not possible via traditional thermal route.² The understanding of how the palladium is modulated by the phosphine ligands is essential for an efficient synthesis. In this context, key steps for understanding the catalytic cycle were investigated.³ Reactivity threshold analysis indicated the presence of a maximum volume of phosphine is required to complete the catalytic cycle, which corroborates the literature of the requirement for a bisligated palladium.⁴ The correlation of the reactive phosphines indicated a univariate trend between yield and the non-covalent interaction London dispersion potential.⁵ NMR and DFT studies are being carried out to full elucidate the mechanism.



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