

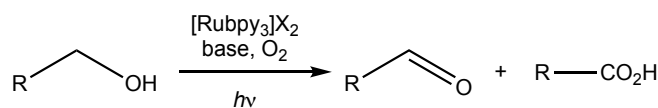
# COMPUTATIONAL STUDIES OF VISIBLE LIGHT PHOTOREDOX CATALYTIC REACTIONS

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Radical chemistry is a powerful and versatile tool for synthetic chemistry. Single electron transfer processes offer complimentary reactivity to two-electron or polar reactions, due to the open shell reactive species that undergo chemical reaction through otherwise difficult to access pathways. The use of radical chemistry in synthesis has become more prevalent in part due to an improved appreciation of the usefulness of photochemistry, which has led to the area of photoredox catalysis. Visible light mediated photoredox catalysis has given rise to a wide variety of synthetic processes including late stage functionalization, carbon-carbon and carbon-heteroatom bond formation reactions.<sup>[1]</sup> Photocatalyzed radical reactions also benefit from generally occurring under mild conditions such as ambient temperature, low catalyst loading, and also exhibiting good functional group tolerance.

Density functional theory (DFT) is a widely used computational method that supports the understanding of a diverse array of synthetic processes. Whilst computational methods have been used to study a variety of catalytic processes, use in visible light promoted reactions remains relatively uncommon.<sup>[2]</sup> This theoretical study provides insight into the mechanism of transition metal catalyzed photoredox oxidation reactions such as that described in the Figure.



**Figure.** Photoredox oxidation reactions

Elucidating the reaction mechanism is important to the design and execution of new synthetic reactions and will assist in deepening the understanding of catalyst reactivity. Of particular importance to this project is to better understand both the chemo- and regio-selectivity of photoredox oxidation reactions.

## References

- 1) M. H. Shaw, J. Twilton, D. W. C. MacMillan, *J. Org. Chem.* **2016**, *81*, 6898
- 2) T. B. Demisse, J. H. Hansen, *Dalton Trans.* **2016**, *45*, 10878