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Computational studies on Ni-catalyzed C–O bond activation of esters

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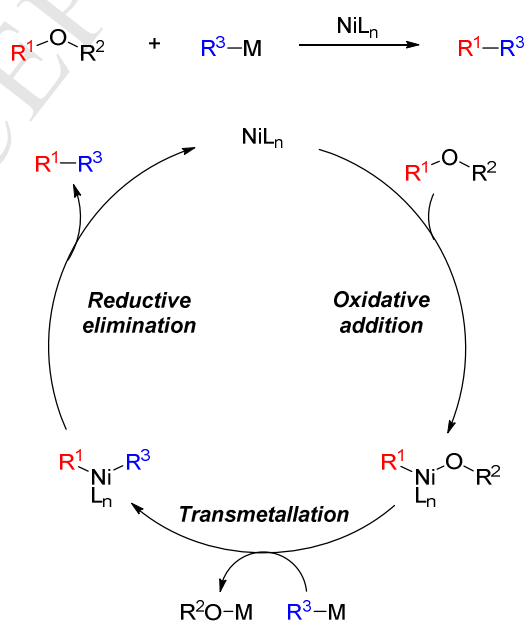
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Abstract: Ni-catalyzed C–O bond activation of esters provides an unprecedented synthetic approach to utilize esters. To understand the mechanistic details of the Ni-catalyzed C–O bond activation, computational chemists have dedicated remarkable efforts to elucidate the origins of reactivities and selectivities of this important process. In order to provide a general perspective of this exciting area, this review summarizes the recent advances of the computational studies involving Ni-catalyzed C–O bond activation of esters. The mechanistic models of C–O bond cleavage are categorized in three types, and the key mechanistic information regarding the control of reactivities and selectivities is presented.

Keywords: nickel catalysis; C–O bond activation; reaction mechanism; reactivity and selectivity; density functional theory calculations

1. Introduction

Ni catalysis has emerged as a powerful approach to facilitate synthetic transformations involving C–O bond cleavage. [1-2] Through the elegant design of ligand and nickel complex, Ni-catalyzed C–O bond cleavage has been realized on a wide array of substrates, which includes esters, [3] carbamates, [4] sulfamates, [4d, f, g, 5] phosphates, [6] phenolates, [7] and ethers. [1g, 8] This allows a facile way of generating organonickel species, and a decade of synthetic development has furnished a series of remarkable transformations to achieve C–C, [3d-g, 3i, 3k-m, o, 4a-e, 4g, 7-8] C–N, [3c, r, s, 4f, h, 5c, d, h, 6b, 8d] C–B, [3h, 8q, r] C–Si, [3h, 8q, r] C–H, [4i, 8e-g, 8m] C–P [3n, p] and C–Sn [3q] bond formations (Scheme 1).



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