Quantum mechanical rapid prototyping (QMRP) of rhenium based catalysts for methane activation

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The computational analogue to combinatorial chemistry, quantum mechanical rapid prototyping (QMRP), has been used to screen a large number of possible rhenium based catalysts of the type \((L_1)(L_2)\text{Re(OH)(OH}_2\)). We have begun by limiting the species to bidentate ligands of the type acac, catechol, ethylenediamine, glycol and picinolate, as well as the sulfur and phosphorus analogues. This choice of ligands has allowed us to explore reactivity as a function of oxidation state \([\text{Re(I)}, \text{Re(III)} \text{and Re(V)}]\), charge (neutral, cationic and anionic species are considered) and ligand type (first row vs. second row comparisons), as well as identify a few systems worthy of more detailed study with experimental collaborators.