Computational search for catalytic materials potentially offer a highly accelerated path towards addressing some of our time’s most pertinent technological and societal challenges. The systematic introduction of linear energy relations as a dimensionality reduction tool in catalyst searches lead to what is now referred to as the “descriptor-based search approach”. This approach has been successful in finding leads for novel heterogeneous catalysts and electro-catalysts. Many challenges still persist for the descriptor-based search approach to become a standard tool for “catalysts engineering”. Ways to improve the reliability of catalyst search studies will be discussed, including the introduction of adsorbate-adsorbate interactions in mean field microkinetics, corrections for systematic electronic structure errors, on known benchmarks, introducing uncertainty estimates, and establishing materials database infrastructure. [1]
