In silico search for novel methane steam reforming catalysts

This paper demonstrates a method for screening transition metal and metal alloy catalysts based on their predicted rates and stabilities for a given catalytic reaction. This method involves combining reaction and activation energies (available to the public via a web-based application 'CatApp') with a microkinetic modeling technique to predict the rates and selectivities of a prospective material. This paper illustrates this screening technique using the steam reforming of methane to carbon monoxide and hydrogen as a test reaction. While catalysts are already commercially available for this process, the method demonstrated in this paper is very general and could be applied to a wide range of catalytic reactions. Following the steps outlined herein, such an analysis could potentially enable researchers to understand reaction mechanisms on a fundamental level and, on this basis, develop leads for new metal alloy catalysts.

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