Catalyst Informatics Study for the Selective Functionalization of Methane

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Abstract:
The selective functionalization of methane (CH_4) has attracted increased attention in recent years because of its scientific interest and industrial importance.[1-3] There is a need for heterogeneous catalysts that can directly convert CH_4 into useful chemicals. On active metal surfaces such as Ni (111), CH_4 is sequentially dehydrogenated to CH and C in exothermic processes.[4] We have considered a difficult process to obtain useful C_2 products such as C_2H_4 and C_2H_6 directly from CH_4. Considering two properties required for a methane conversion catalyst, i.e., reactivity and selectivity, alloy surfaces that energetically stabilize CH_2 and CH_3 species more than CH and C species would be suitable for the direct methane conversion to C_2H_4 and C_2H_6.[5] An exhaustive screening of alloys satisfying this condition is carried out by using first-principles calculations. MgPt is predicted to be one of the most useful catalysts. The activity of Pt is moderately suppressed on its surface, due to Mg, and CH_3 and CH_2 species get more stable than the CH and C species. It is predicted from the calculations that the C-C coupling reaction of two CH_2 species adsorbed on the surface will produce ethylene with a low activation barrier. Experimental verification is carried out by preparing MgPt alloy in collaboration with experimental groups.[5]

References:

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