Finding the solids that are the best catalysts for a given reaction is a daunting task due to the large number of combinations and structures of multicomponent Surfaces. In addition, it is not only the reaction rate that needs to be optimized: the selectivity, durability, and cost Must also be taken into account. Here we propose a computational screening approach and apply it to design a new metal alloy catalyst for the methanation reaction (CO+3H(2)->CH4+H2O). (c) 2006 Elsevier Inc. All rights reserved.