Toward computational screening in heterogeneous catalysis: Pareto-optimal methanation catalysts

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.
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 3.38 SNIP 2.193
Web of Science (2010): Impact factor 5.415
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.965 SNIP 2.135
Web of Science (2009): Indexed yes
Scopus rating (2008): SJR 3.123 SNIP 2.164
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 3.15 SNIP 2.138
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 3.137 SNIP 2.043
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.99 SNIP 2.17
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.623 SNIP 2.015
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.407 SNIP 1.783
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.317 SNIP 1.771
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 2.829 SNIP 1.873
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 2.344 SNIP 2.156
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 2.309 SNIP 1.951
Original language: English
DOIs:
10.1016/j.jcat.2006.02.016
Source: orbit
Source-ID: 195251
Research output: Research - peer-review › Journal article – Annual report year: 2006