The Catalyst Group Resources
(a member of *The Catalyst Group*)

Gwynedd Office Park • P.O. Box 680 • Spring House, PA 19477 • Phone: 215-628-4447 • Fax: 215-628-2267
E-mail: tcg@catalystgrp.com • Web Site: www.catalystgrp.com

PRESS RELEASE . . .

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Advanced Catalyst Design II
(completed August 2006)

Recent advances in catalysis have presented researchers with powerful tools that have enormously increased the opportunities for catalyst design.

In a detailed and comprehensive report which covers the application of these tools to catalyst design, focusing on surface science techniques, nanotechnology, computational modeling and high throughput methods, members of The Catalyst Group Resources (TCGR) **Catalytic Advances Program (CAP)** have exclusive access to a state of the art report. In each of these areas, the report covers the technology's application, recent developments and remaining hurdles and challenges.

Entitled ***"Advanced Catalyst Design II,"*** the report is authored by leading industrial and academic experts and is peer reviewed. Some of the noteworthy findings in this analysis include:

- **Catalyst Design Based on Surface Science and Nanomaterials:** The isolation and characterization of relevant surface species represents one of the most important contributions of surface science to catalysis. Surface science studies have shown that adsorbate surface bonds are localized, which means that surface chemistry can often be predicted based on studies of organic or organometallic chemistry. Unstable and transient surface species such as alkyl groups can be prepared using appropriate precursors. The carbonaceous deposits formed on metal catalyst surfaces during hydrocarbon reactions can also now be characterized by surface spectroscopy under *in situ* conditions.

- **Computational Catalyst Design:** Computational modeling is now providing the type of detailed information on catalytic reactions that is essential for rational catalyst design. Future efforts will likely focus on: (a) the application of new semi-empirical methods to the rapid computational screening of potential catalysts; (b) the development of meso/macroscale models for catalysts using information from molecular simulations; (c) the development of QSAR models to identify key features that can be used to design improved catalysts.

- **Catalyst Design Using High Throughput Methods:** A methodology for the construction of QSARs for solid catalysts has recently been developed and has been successfully applied to the discovery of catalysts for propylene oxidation. QSARs could be useful in defining intellectual property in patents, as a class of catalysts could be more securely patented using descriptors than with structural variations alone.

Additional technical reports issued on a members-only basis in 2006 include: ***Advances in Catalysis for Fuel Reforming and the Water Gas Shift Reaction*** and ***Catalysis for the Upgrading of Heavy Oil***.

To view the report's complete Table of Contents, List of Figures and List of Tables, please visit http://www.catalystgrp.com/capprogram.html. For further information on these reports and the membership-driven **Catalytic Advances Program (CAP)**, please contact Mr. John J. Murphy (jjm@catalystgrp.com) or call 215-628-4447.

The Catalyst Group Resources (TCGR), *a member of The Catalyst Group, is dedicated to monitoring and analyzing technical and commercial developments in catalysis as they apply to the global refining, petrochemical, fine/specialty chemical, pharmaceutical, polymer/elastomer and environmental industries. The Catalyst Group Resources' assessment is based on information obtained from the public domain as well as internal sources and industry interviews. TCGR's analysis will report factual information, as well as hypotheses/interpretations based on this information, in order to derive a reasonable set of expectations. Factors could cause actual results to differ from our forward-looking statements and The Catalyst Group Resources undertakes no obligation to publicly revise these forward-looking statements to reflect events or circumstances after the date hereof.*