

# Computational Design of Catalysts

The U.S. chemical, biochemical and pharmaceutical industries are the world's largest producer of chemicals, ranging from "wonder" drugs to paints to cosmetics to plastics to new more efficient energy sources. All of these industries rely for their financial well-being on their ability to produce new products in an **efficient, cheap, and environmentally clean** process, with a minimal number of undesirable side products. A key ingredient in nearly all such industrial processes is a type of chemical called a **catalyst**. A catalyst's role is to make a chemical reaction that produces a desired product proceed much more efficiently than it otherwise would. A catalytic converter in an automobile is one example. In biological systems, catalysts are called enzymes. As the design of new products becomes ever more sophisticated, the design of new catalysts grows rapidly in importance. While Mother Nature is very effective at designing catalysts, we are decidedly less so. The most common approach to catalyst design is Edisonian: Try something. If it works, try to improve upon the design by systematically changing the chemical nature of the catalyst. If it doesn't work, try something else. This approach is highly intensive, both in terms of time and expense, and frequently, it doesn't work. In addition, catalysts developed using this approach often produce undesirable by-products, and the catalyst itself may pose an environmental hazard (see the figure). For many catalytic processes it is still unclear just how the catalyst works. A much more desirable approach to catalyst design is therefore to analyze, at the molecular level, exactly how catalysts function. Without this information, it is impossible to "tune" the catalyst to have the desired ef-



fect. Since even the most sophisticated experimental techniques are unable to provide the details of the chemical reactions occurring at the surface of a catalyst, the required understanding is only possible by taking advantage of high performance computational hardware and software.

The true computational design of practical catalysts for industrial and commercial applications will require the ability to predict, at the molecular level, the detailed behavior of the large, complex molecules and materials involved in catalytic processes. The level of detail is not available from experiments, and it is not feasible on currently available computer hardware. For example, to simulate the platinum catalyst in a car's catalytic converter requires the model to include hundreds to tens of thousands of platinum atoms. A realistic simulation of the actual process in a car engine would take decades on today's computer hardware. The design of new catalysts simply cannot wait this long if the US chemical and pharmaceutical industries are to remain competitive. However, recent advances in computational molecular and materials science combined with terascale computers—computers capable of trillions of arithmetic calculations per second—can potentially increase the speed of this design process by several orders of magnitude. These new computational capabilities will revolutionize the chemical industry, turning the "art" of catalysis creation into the "science" of catalyst design.

To achieve this goal will require the development of a new generation of computational capabilities consisting of terascale computers; high-performance modeling software; problem solving

environments to enable the use of the computers and modeling software; and databases for capturing the knowledge gained in the simulations. Developing these capabilities will be multidisciplinary efforts—theoretical and computational molecular and materials scientists working in close cooperation with computer scientists and applied mathematicians to develop the modeling software, and then these computational scientists working closely with computational chemical engineers to turn promising new catalysts into a practical chemical manufacturing processes.