Computational Design for Catalysis and Energy Materials

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During the past decade the theoretical description of science and engineering phenomena has undergone a dramatic development. Today's advances in computational capabilities and algorithms make it possible to design new materials with properties tailored to specific applications within the detail and accuracy required for computational results to compare with experiments. We have guided experimental efforts, using the information of new materials at the atomic and molecular level obtained by the state-of-the-art theoretical methods such as density functional theory calculations. Theoretical guidance based on this has played a valuable role on novel chemical processes and important technological advances by directing experimental efforts to the most promising of many possible materials that can be considered. The major focus here is on the discovery of materials with desired properties for a wide range of important applications, including catalysts for the conversion of syngas, chiral surfaces for manufacturing enantiopure drugs, and electrode/electrolyte materials in solid oxide fuel cell.