Modeling of Ceria Based Particlesand Analysis of Their Surface Chemistry

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Computer simulation is one of the main research tools to find and develop new materials for various purposes such as low price, high activity, and durability on diverse reaction conditions. Until now, most experimental approaches mainly have used to "trial and error" method to develop new particle-based materials, which makes difficulties in massive material screening due to the high cost for those experiments and the limitation of instruments.

In this regard, first principles-based density functional theory (DFT) calculations can provide a deep understanding of material properties at the atomic scale and massive material screening with high simulation accuracy and moderate computational cost by using parallel computing and advanced algorithm.

In this symposium, I will present (1) a brief introduction of DFT, (2) applications of DFT to investigate physical, chemical, and catalytic properties of ceria-based nanoparticles, and (3) experimental demonstrations of theoretical prediction with several examples.