# Unraveling the Potentials of Non-precious Metal-based Catalysts through Computational Materials Design


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| Keywords | Computational Materials Design, First Principles Calculation, Metals, Catalysts, Energy, DFT, Metal Alloys, Metal Oxides |


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| Technical Support Skills | · DFT-based computational software, e.g. VASP, Gaussian<br>· Data plotting and atomic visualization software, e.g. GNUplot, VESTA, Chemcraft<br>· Technical writing |

## Research Contents — First Principles-based calculation on the reactivity of metal-based surfaces

The process of research method that we are employing follows the Computational Materials Design paradigm (Fig. 1). In this scheme, basic understanding of a physical phenomenon, particularly in reactions, is attained through analysis of molecular interaction at the atomic level though first principles-based calculations and investigations. From the derived knowledge, significant parameters and factors relevant to a reaction/phenomenon of interest is identified. And from this, materials design is carried out by altering material physical properties. The effectiveness/reactivity of the newly derived materials will then be analyzed using first principles calculations, and the cycle continues until the desired material improvement is attained.

Some of the previous researches have been conducted using First principles-based analysis through density functional theory (DFT) involves: (1) analysis of $H_2O$ molecular interaction on a photocatalyst material such as $TiO_2$ and g-$C_3N_4$ (Fig.2a), (2) investigation of O ion conduction in a ceramic-based ion conductor, such as $Pr_2NiO_4$, for finding efficient electrolyte material for solid oxide fuel cell (SOFC) (Fig. 2b), (3) oxygen reduction reaction (ORR) analysis on a carbon-based cathode catalyst for proton exchange membrane fuel cell (PEMFC) (Fig. 2c), and (4) understanding of the switching mechanism in resistance random access memory (ReRAM) device material such as $HfO_2$ (Fig. 2d).

With the advent of technological advancement towards the nano-particle size, we will employ CMD to design metal-based and metal-oxide-based nano-catalysts for varied reactions related to technology for finding alternative source of energy, and initiatives for preservation of the environment. We hope that through this we will not only understand the unique properties of metals at the nano-particle size but also develop novel materials

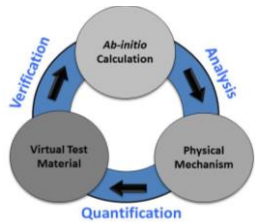


**Figure 2**. Computational Materials Design (CMD)

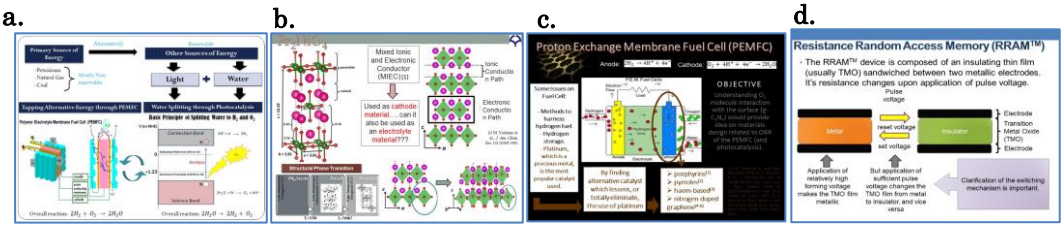


**Figure 2**. Previous first-principles based researches employing CMD.

## Available Facilities and Equipment

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