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ENHANCING QUALITY RESEARCH & INNOVATION for SOCIETAL DEVELOPMENT

P-78 Applying Computational Materials Design (CMD) toward Efficient Hydrogen Production from Water

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Hydrogen is probably the most promising solution to our global energy problems for the future. However, in order to support the developing hydrogen economy, efficient processes for hydrogen production and storage become necessary. Now a days, the hydrogen production is a large and growing industry. Globally, some 50 million metric tons of hydrogen are produced in a year. The growth rate is around 10% per year.

Hydrogen can be produced using fossil fuels via steam reforming or partial oxidation of natural gas and by coal gasification. Produced in this fashion, hydrogen will generate less CO_2 than conventional internal combustion engines (including the emissions during fuel production, delivery, and use in the vehicle), and thus contributes less to global warming. It can also be produced via electrolysis using electricity and water, consuming approximately 50 kilowatt hours of electricity per kilogram. This method is still expensive.

The direct thermal splitting of water, $2H_2O \rightarrow 2H_2 + O_2$, which does not generate CO_2 and produces highly pure hydrogen, requires temperatures in excess of 2000 ^oC thus making its practical implementation very challenging. Here by using *ab initio* calculations, we introduce a simple technique to find the best catalyst that can decrease this direct thermal splitting. As an illustration, we consider cyanocobaltate complexes. These materials are well known for their effectiveness in binding and releasing O_2. By using density functional theory, we calculate the potential energy surface (PES) of a reaction i.e., $2H_2O \rightarrow 2H_2 + O_2$ on these materials, and determine the energy barrier (which can be related to the direct thermal splitting) for water dissociation of this reaction. We found the energy barrier for the water dissociation decreases significantly using cyanocobaltate complexes compared to the case of two water molecules in the isolated case.

P-81 SMS and MMS to Enhance an Integrated Medical Emergency Model for Malaysia

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The current situation of Malaysian hospitals, healthcare and emergency centers shows that it has no unified medical information and healthcare systems. Several systems are still paper-based and stand alone systems. Although the mobility and Multimedia facilities such as SMS and MMS are very important and widely used now in many applications but it still poorly or not used in such systems. This research work focuses on enhancing the development of an integrated Medical Emergency with the SMS and MMS facilities. The proposed system: uses SMS to guide patient or authorized user to the nearest hospital or health care center, search for hospitals and broadcast important health related information. MMS is used to offer the capability of sending multimedia information such as text, pictures, voice and video to the related medical emergency staff. A medical emergency call center module is created to handle emergency calls. A prototype implementing for the proposed features is created using open source tools. Sample of the results are provided.