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A first-principles study on effects of electric field on heterogeneous catalysis

Improving the selectivity of chemical reactions is arguably the primary challenge in developing an efficient catalyst in catalysis. Electric fields can be used to adjust the thermodynamics of chemical reactions as like temperature and pressure, and it can control selectivity through the field–dipole interactions. Therefore, we attempt to develop an efficient catalyst for the selective methane conversion process and the Iodine reduction reactions as these are essential in solving the environmentally sustainable issues and the energy crises. As indicated in our earlier study, IrO_2 (110) surface can activate methane at a very low temperature. However, due to the strong reactivity of IrO_2, the adsorbed methane will be completely oxidized, so it is not advantageous to form a value-added chemical on IrO_2. Hence, to adjust the reactivity of IrO_2, here we considered the partial oxidation of methane in the presence of external electric field. Our results demonstrated that we could adjust the adsorption and desorption of the species on the surface with the external electric field. The most favorable reaction pathway is the production of surface formaldehyde by applying a positive external electric field. Likewise, finding and improving the performance of Pt free counter electrode(CE) in DSSCs is widely researched in energy conversion/storage fields. Hence, here we also investigated the influence of an electric field on the adsorption stability and the possible reduction reactions of I_2 molecule on B-doped, N-doped, B-N co-doped, and pristine graphene nanosheets. Our results show that applying an electric field can significantly enhance the I_2 adsorption and can alter the kinetic properties of the reduction reaction on N-doped graphene under a negative electric field, which will be a potential counter electrode replacement for Pt in DSSC devices. These results demonstrate that the catalytic activity of a catalyst can be effectively controlled by means of the electric field.

Speaker Biography

Jyh-Chiang Jiang graduated from National Taiwan University in 1986 with a B.S. in Chemistry and received his PhD in Chemistry in 1994 from the National Taiwan University. After working as a postdoctoral fellow at IAMS, he joined the faculty of National Taiwan University of Science and Technology (NTUST) in 2001. He has more than 170 papers in peer-reviewed journals. His research has also resulted in 4 patents and has been serving as an editorial board member of Scientific Reports.

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