DIPARTIMENTO DI CHIMICA, BIOLOGIA E BIOTECNOLOGIE

UNIVERSITÀ DEGLI STUDI DI PERUGIA

SEMINAR

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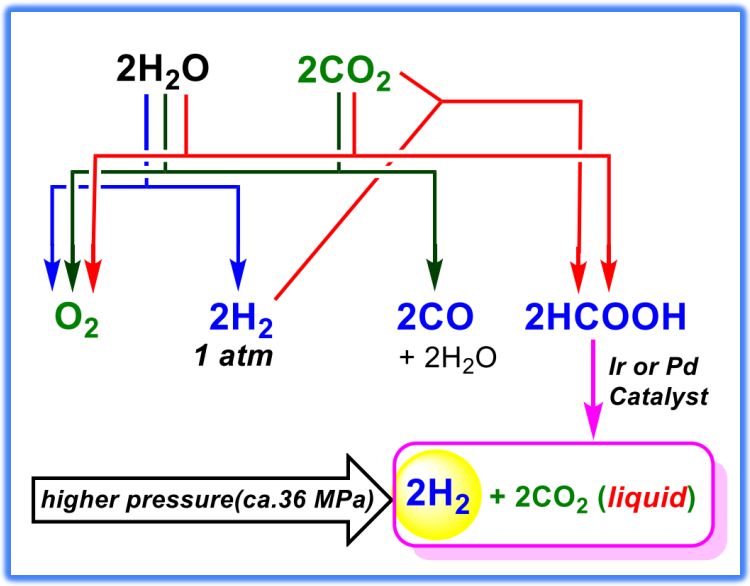
Mechanistic Studies on Water Splitting and CO_2 Reduction Towards Solar Fuels Production



On Monday 5th September 2022

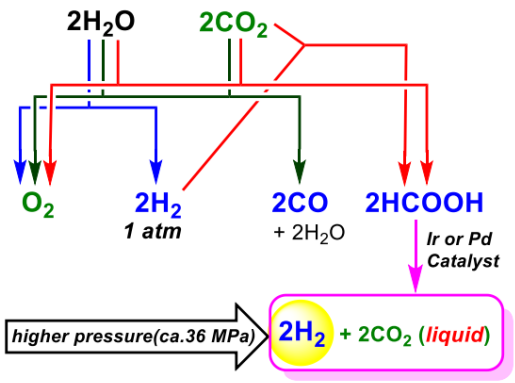
11:00 am - Room G

Department of Chemistry, Biology and Biotechnology – Via Elce di Sotto 8

Host: Prof. Alceo Macchioni

DIPARTIMENTO 2018 di ECCELLENZA 2022 AMIS project

Among various approaches attempting to develop renewable energy sources, solar hydrogen production via water splitting has received an increasing attention in relation to the recent advancement in the hydrogen fuel cell technology. The combustion energy after storing two reductive equivalents decreases in the order of H_2 (**he**) > CO (0.99**he**), HCHO (0.99**he**) > HCOOH (0.89**he**) > CH_3OH (0.85**he**) > CH_4 (0.78**he**) (**he**=286 kcal/mol). The source of electrons and protons can be produced in the artificial photosynthetic water oxidation process ($2H_2O + 4h\nu \rightarrow O_2 + 4H^+ + 4e^-$). Among these fuels, only formic acid and methanol are liquid and possess superior characteristics from a viewpoint of energy density together with the feasibility in refueling and transportation in ambient conditions. Further, formic acid has a remarkable potential as a source of ***high-pressure*** **H_2** because of its reversible conversion capability: $HCOOH \leftrightarrow H_2 + CO_2$ (ΔG = -12 kcal/mol; see figure, right). The production of $\{O_2+2HCOOH\}$ is advantageous owing to the spontaneous separation of the two products into the gas and aqueous phases, while the production of $\{2H_2+O_2\}$ or $\{2CO+O_2\}$ yields a flammable gas mixture. With these perspectives in mind, our recent interests still concentrate on the basic studies towards the improvement of our understanding on the mechanisms of water reduction and CO_2 reduction on various transition metal molecular to heterogeneous catalysts.[1-5] We succeed to develop and investigate the environmentally friendly photocatalytic CO_2 reduction in fully aqueous media.[1,2] We have advanced our understanding on the mechanisms of catalytic CO_2 reduction by DFT.[2,3] We have also advanced our studies on two-electrode solar water splitting systems which permit H_2 separation at a dark cathode.[4] A quite new topic in our group is the project on the mechanistic studies of electrocatalytic hydrogen evolution reaction by platinum subnanoclusters.[5]



1. A. Call, M. Cibian, K. Sakai, et al., ***ACS Catal.*** **2019**, *9*, 4867-4874.
2. X. Zhang, K. Yamauchi, and K. Sakai, ***ACS Catal.*** **2021**, *11*, 10436-10449.
3. Y. Sakaguchi, A. Call, K. Yamauchi, and K. Sakai, ***Dalton Trans.*** **2021**, *50*, 15983-15995.
4. H. Ozawa and K. Sakai, ***AsiaChem*** **2021**, *2*, 80-87.
5. K. Kuge, K. Yamauchi and K. Sakai, ***ChemRxiv***, April 1,**2022**.