Journal of Advances and Scholarly Researches in Allied Education
Vol. 16, Issue No. 4, March-2019, ISSN 2230-7540

Model Systems in Heterogeneous Catalysis: A Review

Mr. Saurabh Kumar*

Research Scholar, Department of Chemistry, Singhania University, Rajasthan

Abstract* – *Heterogeneous catalysts, frequently working beneath tremendously robust circumstances, are important to development of huge range of chemicals that rely on our modern civilization. Because of their technological advantages, most industrial catalytic processes use heterogeneous catalysts. Heterogeneous catalysis currently covers closely 80 % of the share of the global market. Heterogeneous catalysis for cost-effective and sustainable industrial application and storage is one of the main solutions and processes. Highly efficient & stable heterogeneous catalysts are being sought and explored as a new frontier to address the energy and environmental challenges we face. Fortunately, increasing nanotechnology provide one of solutions through growth of nanocatalysts with maximum activity, selectivity & stability.

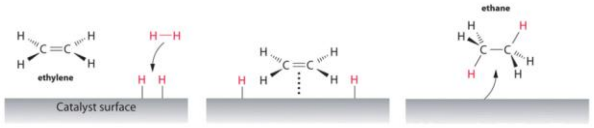
Keywords: Catalysis, Selectivity, Nanoparticles, Adsorption, Reaction.

- x -

I. INTRODUCTION

The catalyst is in different phase from reactants in heterogeneous catalysis. In a physical function termed as adsorption, at least one of reactants interacts with solid surface so that a chemical bond in reactant is unstable and then breaks. Poisons are compounds that bind irreversibly to catalysts, prevent adsorption of reactants and therefore reduce or kill the efficiency of the catalyst. The interaction of hydrogen gas with a metal surface, like Ni, Pd, or Pt, is an example of heterogeneous catalysis. The hydrogen-hydrogen bonds break down and release particular adsorbed hydrogen atoms on metal surface, as presented in part (a) in Figure 1.

Because adsorbed atoms can travel on surface, 2 hydrogen atoms can collide & form hydrogen gas molecule that can then exit surface in reverse function termed as desorption. Adsorbed H atoms are considerably more reactive on a metal surface than a molecule of hydrogen. Since relatively strong H–H bond has already been broken, energy barrier on catalyst surface for most H2 reactions is significantly lower. Ethylene hydrogenation in a heterogeneous catalyst. When the catalyst surface is adsorbed by a molecule of hydrogen, the H-H bond breaks and new M-H bonds are formed. Less reactive than gaseous H2 are the single H atoms. When an ethylene molecule interacts with surface of catalyst, it reacts in a step-by-step system with the H atoms to eventually create ethane that is produced.



(a) Hydrogen (H_2) adsorbs to the catalyst surface (M) to form adsorbed H atoms.

(b) Ethylene (C_2H_4) adsorbs to the catalyst surface.

(c) Ethylene reacts with adsorbed H atoms to give the product ethane (C_2H_6).

Figure 1 demonstrates a hydrogenation process in which hydrogen atoms are added to an alkene's double bond, such as ethylene, to give a product containing C–C single bonds, in this case ethane.

In the food industry, hydrogenation is used to turn vegetable oils, consisting of long alkene chains, into more commercially viable solid derivatives containing alkyl chains. For example, hydrogenation of some of double bonds in polyunsaturated vegetable oils creates margarine, a material with a melting point, consistency, and other butter-like physical properties. Heterogeneous catalysis is kind of catalysis in that catalyst phase varies from the reactant or material phase. Contrasts to homogeneous catalysis where in the same step there are reactants, products and catalysts. Phase distinguishes among not only components of solid, liquid and gas, but also immiscible mixtures and wherever there is an interface. Catalysts are useful because, without being used, they increase rate of reaction and are therefore reusable. Heterogeneous catalysis usually involves catalysts of the solid phase and reactants of the gas phase.

In this case, on surface of catalyst, there is a process of molecular adsorption, reaction, and desorption. The reaction rate (kinetics) is determined by thermodynamics, mass transfer and heat transfer. Heterogeneous catalysis is significant as it permit faster, large-scale production & creation of selective products. Catalysis affects about 35 percent of world's GDP. Solid catalysts allow production of 90 percent (by volume) of chemicals. There is a heavy dependency on heterogeneous catalysis in chemical and energy industries. The Haber-Bosch process, for example, utilization metal-based catalysts in ammonia synthesis, a significant fertilizer component; 144 million.

Berzelius used the term catalysis in 1835: "Catalysts are sub-stances that cause chemical reactions that would not otherwise occur due to their mere presence.".. Wilhelm Ostwald described a catalyst as: "a material that changes the speed of chemical reaction without appearing in the end products themselves." The Chinese term used for a catalyst means "marriage broker" as well. This brief historical introduction contributes to the catalyst's real meaning. In the stoichiometric formula of the reaction, a catalyst involved in a reaction does not exist.

For an assigned reaction, its effect is to increase the velocities of the reaction for an assigned temperature or to decrease the temperature at which the reaction reaches a defined frequency. Without thermodynamically unstable intermediate product for simple reactions, this ensures that the catalyst operation is to raise both the velocities of the reaction (forward kf and backward kb) in such way that the ratio kf= kb does not alter. Because of this, the equilibrium achieved with a catalyst is simialr when there is no catalyst. It is sigificant to note that a thermodynamically impossible reaction can not be triggered by the catalyst.

His behavior is subject to thermodynamic laws at all times. The "speed-up" obtained using a catalyst is due to the reduction required for a particular reaction of activation energy E (see Fig.2). For the most part, we find a solid catalyst: a lower reaction velocity means a higher velocity constant according to the "transition state principle".

$$k_v = \frac{kT}{h} e^{4G^{=}=RT} \qquad (1)$$

Where k is the constant of Boltzmann, h is the constant of Plank, T is the temperature, R is the constant of gas and 4Gz is the free energy of the activated state. A higher kv means a lower free energy of 4Gz for catalyzed reaction for a fixed temperature. And

$$4G^{z} = 4H^{z} \quad T\,4\,S^{z} \qquad (2)$$

And for catalyst reaction 4Sz is less than the same quantity for the non-catalyst reaction as the particle bound to the catalyst surface loses some degree of freedom. It means that the 4Hz must be lower in order to have a better 4Gz relative to the non-catalyzed reaction. From the transition state theory, we learn that 4Hz= Ea does not change the number of molecules in the reaction, which explains the reduction of activation energy (see Fig. 2).

Based on the chemical cycle of catalyst & reactants, it is possible to define the form of catalysis different:

Homogeneous Catalysis : The catalyst is in similar as reactants & no phase boundary exist.

Heterogeneous Catalysis : There is phase boundary separating catalyst from reactants.

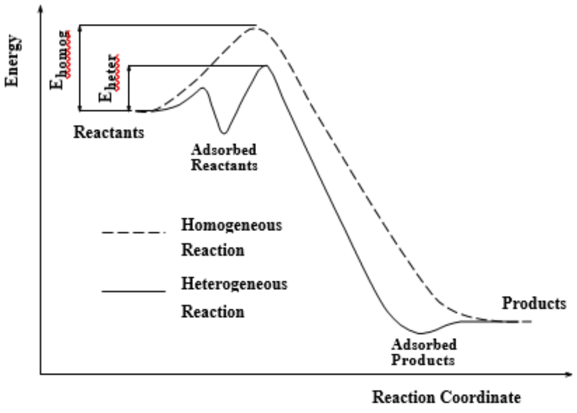


Figure 2. Energy reaction path for heterogeneous and homogeneous reaction.

A gas ow past a solid wall belongs to 2nd case: reactants are gas chemical species & wall is catalyst.

II. MODELLING HETEROGENEOUS CATALYSIS

A scheme representing elementary steps involved in heterogeneous catalysis can be shown as follow:

1. diffusion of reactants to surface;
2. adsorption of reactants at surface;
3. chemical reactions on surface;
4. desorption of products from surface;
5. diffusion of products away from surface.

Each of these phases has a different speed, and the slower speed is the rate of system determination. Steps 1 & 5 are typically fast; if the catalyst is very e user, there are exceptions. The limit for the catalytic reaction rate is the sum of reactants going to the wall and the surface reaction rate is independent of the surface's kinetic properties. This is the case with catalysis of "guided diffusion." Space vehicle coatings TPS are being studied to have very poor catalytic efficiency, to reduce the surface heat ux as much as possible duetore-combination results.

1. Adsorption

Adsorption is the creation of a bond between the atom and the solid surface, or the molecule. We are speaking about physisorption (physical adsorption) when the bond between surface & gas particles is induced by the forces of van der Waals (forces of inert atoms and molecules). The forces involved are electrostatic forces for molecules with permanent moments of dipole, induced polar at-tractions for readily polarizable molecules, dispersion forces for non-polar atoms and molecules (forces attributable to electron density fluctuation). The strength of these bonds depends on the adsorbed gas's physical properties and is related to gas's boiling point (or condensation).

Physisorption is not highly dependent on the solid's chemical composition. The energy of the particle-surface bond is small (10-50 kJ / mole) and the bond is only significant at low temperatures (100-300 K): the gas is extracted more or less completely as the temperature rises. The importance of this method of adsorption in heterogeneous catalysis lies in the fact that it can be a precursor to chemisorption. Chemisorption properties of the solid surface. A solid's surface may have properties that differ markedly from those of bulk solid since unsaturated bonds exist on the surface.

In addition, a surface atom is not in the same condition as a "bulk" atom, as it does not have its complete neighbors complement. It refers to both a covalent solid (such as SiO_2, SiC) and an ionic solid (such as N aCl). An easy way of understanding this situation is to think about an ideal crystal fracture: the fracture sides are new surfaces where atoms that used to be inside the bulk are now "dangling" bound surface atoms. If a free gas atom is near to a solid surface, there is an attractive contact between it and the surface atoms: the atom is drawn to surface & it can be a position, i.e. a physical location corresponding to one of the "dangling" bonds.

The bond formed is a real, normally covalent chemical bond: particle shells are interpenetrated with electron sharing and the bond energy is high (40-800 kJ / mole). Chemisorption takes place until the valences of the unsaturated surface are filled. This explains why, if multilayer physisorption is possible, no more than one layer can be adsorbed by chemisorption even though new species may develop on the surface (e.g. due to metal oxidation). Physisorption and chemisorption are spontaneous (4H < 0), but the latter may have significant energy to activate.

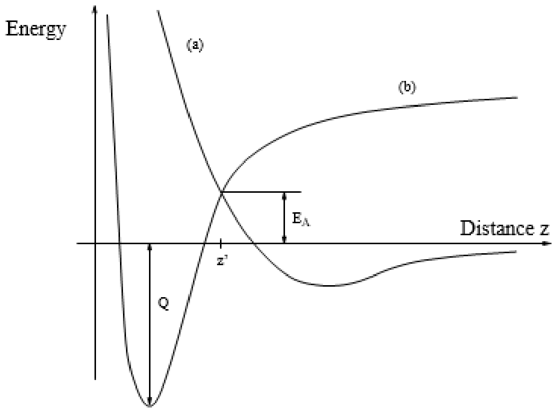


Figure 2. Potential energy curves for adsorption: (a) physisorption of a molecule; (b) chemisorption of two atoms.

2. Reaction

Interesting reactions for hypersonic applications are suggested nations of atoms that form O_2 and N_2 and reactions that generate N O, CO, and CO_2. For heterogeneous catalysis, for order to react catalytically on a solid surface, reacting particles must be chemisorbed. Thus, if physisorption does not play a specific role, chemisorption is a crucial stage in the "preparation" of atoms and molecules for reaction. This mechanism provides a reaction path lower than one of the corresponding homogeneous reaction with an activation energy.

The remaining processes of reaction that we find are the recombination of an atom from the gas and an adsorbed one: the free gas atom hits and interacts with the adatom. The product is a molecule that is recombined. This is called the process of Eley-Rideal (E-R) and a simple scheme is:

$$A + B^* \rightarrow AB^*$$

Where the letters A, B is an atom. The molecule AB is still adsorbed after recombination. The speed of this reaction depends on the gas phase atoms ' partial pressure and the coverage of the surface. We can write on this basis for the phase rate:

$$u_{ER} = k\,[A][B^*]$$

The 2nd mechanism is recombination among 2 adatoms: this is termed as Langmuir-Hinshelwood mechanism (L-H) & schematic representation is:

$$A^* + B^* \rightarrow AB^* + *$$

This type of reaction is obviously possible when adatoms are used over the ground. A way to move adatoms is to "jump" from one potential well to another overcoming a potential Em barrier that is lower than the Ed desorption energy; in addition, particles do not leave the surface entirely during this movement. Em~0.1-0.2 Ed can be found in literature. This value depends on extent of the surface exposure (when it increases), the surface defects and the surface's crystallographic orientation. The existence of the Em energy barrier means that the L-H mechanism is an active system that, with respect to the E-R mechanism, is effective at higher temperature. This is evident in the catalysis involving metal surfaces, when the L-H cycle begins, the recombination coefficient drops sharply.

3. Desorption

There is no chemical bond among surface & molecule after E-R or a recombination of L-H, which is called free desorption. Desorption may not be "immediate" and the molecule may drop well before leaving in a physisorption (see Fig. 3). Desorption is, in any case, a very fast process, and many authors consider reaction and desorption as a single step. The value of this phenomenon lies in the fact that, when the molecule leaves the wall, recombination energy can be left in whole or in part on the surface.

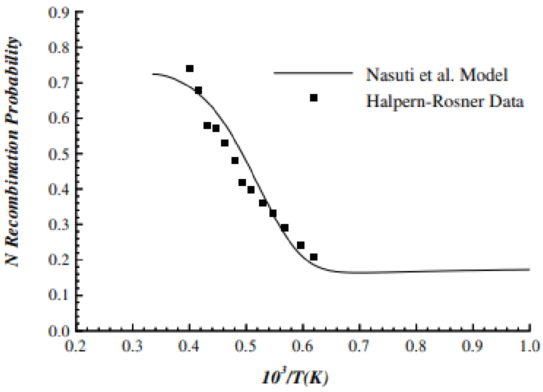


Figure 3. Nitrogen recombination over tungsten: N vs inverse temperature.

The characteristic desorption time is strictly related by the molecular internal energy release mechanism to amount of energy left on the wall. It means that the molecule can either leave surface in an excited state and then "quench" in the gas near the wall, or leave the surface with it in thermal equilibrium. In order to take this phenomenon into account, a chemical energy accommodation (CEA) coefficient is defined as the fraction of the energy supplied to catalyst surface by recombination event:

$$\beta = \frac{q}{D_{AB}\Delta n/2} \qquad (3)$$

Where q is the effective flux of energy to the wall, n is the flux of recombined atoms and DAB is the dissociated energy of the AB molecule. Experimental values indicate a dependence on surface-recombined molecules interaction. If bond is "solid" between the recombined molecule and the ground, there is sufficient time for full accommodation. If the bond is "strong," on the contrary, the molecules easily desorb and the energy left on the wall is smaller.

In theory, significant savings in TPS tend to be feasible if reliable and accurate decision could be made and if a priori it could be "built" based on material properties and the form of recombining atoms. This is ground boundary catalysis still in need of exploration.

4. Thermal Desorption

In addition to the mechanisms described above, we also need to consider thermal desorption. In addition, adsorbed atoms vibrate with the frequency kT / h; these vibrations will detach the atom from the potential well that contributes to desorption at sufficiently high temperatures:

$$A^{*} \downarrow A + *$$

Following transition state theory, the rate of desorption reads:

$$u_{des} = N_a \frac{kT}{h} \frac{e^{\Delta}S}{k_e} - \Delta H/(kT)$$

These are variations between two states (adsorbate-gas) : entropy and enthalpy respectively. Normally 4H should be of simailar order of adsorption energy magnitude. Thermal desorption is necessary at high temperatures because of the latter's high values.

5. Rate Determining Step

We will address the concentrations of heterogeneous phenomena on a standard substrate in the following. That's why we're going to talk about low and high temperatures without any different cations. What we mean for "low" in any case are temperatures not far from normal, and temperatures above 1000 K for "extreme." It would be easier to differentiate between metallic and non-metallic surfaces in a more detailed discussion, but the following discussion is common enough for both cases.

The surface distribution is similar to unity at low temperatures; this is because the mobility of atoms is very small and there is no effective thermal desorption. Under these conditions, it is predicted that the E-R recombination mechanism will be more active for L-H. In addition, there is a very high likelihood that an adsorbed atom will strike. The rate of adsorption is predicted to be higher than the rate of depletion of surface atoms under these conditions:

$$u_{ads} \gg u_{reac} ; u_{des}$$

Thanks to thermal and L-H recombination desorption, the area decreases when the temperature rises. High temperature increases adatomic mobility and hence the probability of recombination. The L-H method is also very successful because at similar time it eliminates two adatoms. Due to the low possibility of a collision between a gas atom and an adatom, the E-R mechanism becomes less successful as surface coverage is small and adatoms are very mobile and difficult "targets" to reach gas atoms. Under these conditions, adsorption may be the rate limiting step:

$$u_{des} ; u_{reac} \gg u_{ads}$$

The previous discussion leads to some additional comments in addition to describing a rate limiting measure. We can see that the molecules produced by a high probability E-R system are more likely to leave the surface in an excited state. Then they would take part of the recombination power with them. This is not the case for L-H recombined molecules, as they would have enough time to leave all the excess energy to the surface and desorb in thermal equilibrium. It would therefore be predicted that the variable will be small at low temperatures and will rise towards unity with increasing temperature.

III. ADVANTAGES AND DISADVANTAGES OF HETEROGENEOUS CATALYSIS

There are numerous of benefits of heterogeneous catalysis. As one aspect, in straightforward manner, heterogeneous catalysts can be isolated from a reaction mixture, such as filtration. It allows easy and effective recovery of costly catalysts, that is significant for industrial production processes.

One drawback of heterogeneous catalysis, however, has to do with catalyst's available surface area. Once the catalyst's surface is completely filled with reactant molecules, reaction cannot proceed until products leave surface and some room is reopened to adsorb or add a new reactant molecule. The adsorption step in a heterogeneously catalyzed reaction is further rate-limiting step for this reason. Nonetheless, overall benefits of heterogeneous catalysis greatly outweigh their drawbacks, as the catalyzed reaction is much quicker than uncatalyzed reaction.

IV. KINETICS OF HETEROGENEOUS CATALYTIC REACTIONS

The catalytic cycle is the catalytic action principle. The mechanism of a catalyzed reaction can be defined by the sequence of the cycle's elementary reaction steps, including adsorption, surface diffusion, adsorbed species chemical transformations, and desorption, and is for deriving reaction kinetics. The transition-state theory is believed to be true for each individual elementary phase. SCHWAB has published an early treatise on the kinetics of heterogeneously catalyzed reactions. ERTL has categorized the different aspects of dynamics of surface reactions and catalysis into five groups in terms of time and duration scales. This approach was very useful for reactor design and system design in chemical engineering. Reaction schemes (kinetic models) assumptions include comparisons between intermediate surface coverage and external variables, an approach that led to the Temkin equation modeling ammonia synthesis kinetics.

Better kinetic models could be established when there were available atomic processes on surfaces and surface species recognition and characterization. A microkinetics approach explains progress of catalytic reaction by modeling the macroscopic kinetics by correlating atomic processes with macroscopic parameters in sense of an effective continuum model. Continuum variables for partial surface coverage are compared by the Langmuir lattice model of a surface consisting of equivalent non-interacting adsorption sites to external parameters (absolute pressure and temperature) at a first approximation.

For the complete sequence of elementary reactions, the formulation of rate laws may usually result in a series of nonlinear coupled (ordinary) differential equations for the concentrations (coverages) of the different surface species involved. The reaction system's temporal behavior under constant continuous-flow conditions can be transient non-stationary. It can be oscillatory or even unpredictable in certain parameter ranges. Local variations in surface coverage may also result in reaction coupling with transportation processes (e.g., particle diffusion, heat transfer).

The consequence of these nonlinear dynamic processes is the creation of spatiotemporal concentration profiles on a mesoscopic scale. Since the lattice model of Langmuir is not really valid, continuum model can explain kinetics of reaction only to a first approximation. Interactions among adsorbed species occur, and non-identical sites are occupied by adsorbed particles, resulting in difficulties in the characterization of the kinetic reaction. In addition to adsorption sites heterogeneity, surfaces may undergo structural transformations. Surface science research offers atomic scale data on these impacts.

As discussed above, the transition-state theory is presumed to be accurate for the levels of individual elementary steps to be defined. This theory is based on the assumption that thermal equilibrium is formed at all stages along the reaction coordinate. So temperature is the only external macroscopic parameter that is important. This statement can only be true if the transfer of energy between all the degrees of motional freedom of the particles interacting with the solid acting as a heat bath is faster than the basic phase causing nuclear motions. The fundamental conditions for chemical transformations are energy transfer processes at the quantum level. Nonlinear dynamics and anomalies are taking place at the atomic and quantum levels were reviewed by ERTL.

V. MOLECULAR MODELING IN HETEROGENEOUS CATALYSIS

Catalytic reaction modeling is implemented at many complexity levels covering multiple length and time scales orders. This varies from a complete description of the dynamics of a reaction to adsorbing–adsorbing interactions to the basic mean-field approximations discussed and macrokinetic models. In a template hierarchy, the different approaches can be portrayed. This section presents widely used models that either explicitly describe the catalytic cycle's molecular actions or are based on the molecular picture. The output of a calculation using a more sophisticated method also serves as the input for a calculation using a less detailed model, energies computed by DFTare often used as parameters in kinetic Monte Carlo and simulations.

VI. PRODUCTION OF HETEROGENEOUS CATALYSTS

The development of heterogeneously catalyzed reactions for chemical production initiated the preparation on a technical scale of the necessary catalysts. Solid catalysts were primarily developed in process companies such as IG Farben and BASF in Germany and Standard Oil Company and UOP in the USA until the end of World War II. Some independent catalyst manufacturing companies were established in the United States, Western Europe, and Japan about ten years later. More than 15 foreign companies are currently developing solid catalysts on a multitonne scale, including: Synetix, Chemicals and Grace, SUD-Chemie Catalyst Group. Therefore, every phase of production and the physical or mechanical properties of all intermediates must be regulated.

Batch procedures are primarily replaced by continuous operations such as precipitation, filtration, drying, calcination, and shaping to achieve better reproducibility of catalyst output. In catalyst production lines, automation of different operations and computer control of different equipment are installed. In the catalyst production process, SPC (statistical process control) and QA (quality assurance) have recently been incorporated. Some companies produce solid catalysts in accordance with ISO Standard, particularly in Western Europe and the USA, which guarantees the customer a standard catalyst performance.

CONCLUSION

Catalysts participate in and increase their rate of chemical reaction. They do not appear in the net formula of the reaction, and during the reaction they are not consumed. Catalysts allow a reaction to proceed through a pathway with a lower energy of activation than the uncatalyzed reaction. Catalysts provide a surface in heterogeneous catalysis to which reactants bind in an adsorption phase. Throughout modern society, heterogeneous catalysis plays a vital role. Since the heterogeneous catalytic reactions occur on the surface and are affected by the different layer atoms of catalysts, the general catalytic surface should be made as wide as possible to interact with the reactant in order to enhance efficiency. At present, heterogeneous catalysis is the most common method for catalysis. This subject was discussed and is covered extensively in the literature. Support materials are important to stability and performance of the catalysts in heterogeneous catalysis.

REFERENCES

1. Ertl G., Kno¨zinger H., Weitkamp J. (eds) (1997). Handbook of heterogeneous catalysis, Wiley-VCH Verlagsgesellschaft mbH, Weinheim

2. Freund H., Goodman D.W. (2007). In: Ertl G, Kno¨zinger H, Schu¨th F, Weitkamp J (eds) Handbook of heterogeneous catalysis, 2nd edn. Wiley-VCH Verlagsgesellschaft mbH, Weinheim

3. Freund H.J., Libuda J., Ba¨umer M., Risse T., Carlsson A.F. (2003). Chem Rec 3: p. 181

4. Schauermann S., Hoffmann J., Johanek V., Hartmann J., Libuda J., Freund H.J. (2002). Angew Chem Int Ed 41: pp. 2532

5. Magg N., Immaraporn B., Giorgi J., Schroeder T., Ba¨umer M., Do¨bler J., Wu Z., Kondratenko E., Cherian M., Baerns M., Stair P.C., Sauer J., Freund H.J. (2004). J. Catal 226: p. 88

6. Doyle A.M., Shaikhutdinov S., Jackson S.D., Freund H.J. (2003). Angew Chem Int Ed 42: p. 5240

7. Doyle A.M., Shaikhutdinov S., Freund H.J. (2005). Angew Chem Int Ed 44: p. 629

8. Sterrer M, Yulikov M, Fischbach E, Heyde M, Rust HP, Pacchioni G, Risse T, Freund H-J (2006) Angew Chem Int Ed 45: p. 2630

9. Hansen K.H., Worren T., Stempel S., Lægsgaard E., Ba¨umer M., Freund H.J., Besenbacher F., Stensgaard I. (1999) Phys Rev Lett 83: p. 4120

10. Borasio M., Rodrigez de la Fuente O., Rupprechter G., Freund H.J. (2005). J. Phys Chem B. 109: pp. 17791

11. Kaichev V.V., Morkel M., Unterhalt H., Prosvirin I.P., Bukhtiyarov V.I., Rupprechter G., Freund H.J. (2004). Surf Sci 566–568: p. 1024

12. Rupprechter G., Kaichev V.V., Unterhalt H., Morkel M., Bukhtiyarov V.I. (2004). Appl Surf Sci 235: p. 26

13. Magg N., Giorgi J.B., Schroeder T., Baumer M., Freund H.J. (2002). J. Phys Chem B. 106: p. 8756

14. Magg N., Giorgi J.B., Hammoudeh A., Schroeder T., Baumer M., Freund H.J. (2003). J. Phys. Chem. B. 107: p. 9003

15. Abu Haija M., Guimond S., Romanyshyn Y., Uhl A., Kuhlenbeck H., Todorova T.K., Ganduglia-Pirovano M.V., Dobler J., Sauer J., Freund H.J. (2006). Surf Sci 600: p. 1497

16. Dupuis A.C., Abu Haija M., Richter B., Kuhlenbeck H., Freund H.J. (2003). Surf Sci 539: p. 99

17. Guimond S., Abu Haija M., Kaya S., Lu J., Weissenrieder J., Shaikhutdinov S., Kuhlenbeck H., Freund H.J., Do¨bler J., Sauer J. (2006). Top Catal 38: p. 117

18. Kaya S., Sun Y.N., Weissenrieder J., Stacchiola D., Shaikhutdinov S., Freund H.J. (2007). J. Phys Chem C 111: p. 5337

19. Kaya S. (2007). Thesis, Humboldt - Universita¨t zu Berlin, Berlin

20. Romanyshyn Y., Guimond S., Go¨bke D., Sturm M., Kuhlenbeck H., Freund H.J., Ganduglia-Pirovano M.V., Do¨bler J., Sauer J., Top Catal (submitted)

21. Magg N., Giorgi J., Frank M., Immaraporn B., Schroeder T., Ba¨umer M., Freund H.J. (2004). J. Am Chem Soc 126: p. 3613

22. Immaraporn B., Magg N., Kaya S., Wang J., Baumer M., Freund H.J. (2004). Chem Phys Lett 392: p. 127

Corresponding Author

Mr. Saurabh Kumar*

Research Scholar, Department of Chemistry, Singhania University, Rajasthan