# Study of Nano-Materials as a Catalyst and its Behaviors

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## ABSTRACT
Study of catalyst in the domain of chemical science is an important material agent which modifies the rate of chemical reaction without changing its own chemical constituents, when catalyst is present in the form of nanomaterial. Nano-material is used as catalyst for increasing or decreasing the rate of chemical reaction under the controlled parameters of environment. Same catalyst for same reactants under different environmental conditions producesdifferent yields.

### Keywords
Domain, Catalyst, Nano-materials

## 1. INTRODUCTION
Nanomaterials also called as nanocrystalline materials, possess grain size of the order of a billionth of a meter. All materials are composed of grains which are usually invisible to the naked eye, varying in size somewhere from 100's of microns (µm) i.e. ($10^{-6}$) to 100millimeters (mm).

Since nanomaterials possess unique, beneficial, physical, chemical and mechanical properties, they show a wide variety of applications which includes -1) Applications in medicines.2) Applications in Nano electronics.3) Applications in Nano mechanics.4) Applications in environmental technology.5) Applications in catalyst.

But,are not limited to the above points.

To continue with let us discuss about nanomaterials as a catalyst with its behavior.

Catalyst is basically that substance which alters(increases or decreases) the velocity of reaction when taken on nanoscale, without itself undergoing any change in mass and composition at the end of reaction and this phenomenon of altering reaction is called as catalysis.

Catalysts are of two types:

1) Positive catalyst: A catalyst which increases the rate of reaction, for example,

$2KClO_3$-----$^{MNO}{}_2$----> $2KCl + 3O_2$

$2H_2O_2$-----$^{Pt}$---------> $2H_2O + O_2$

2) Negative catalyst: A catalyst which retards the rate of reaction, for example,

$2H_2O_2$----$^{H}{}_2{}^{SO}{}_4$------------>$2H_2O + O_2$

$2H_2O + O_2$-------$^{CO}$------------>$2H_2O$

## 2. CHARACTERISTICS OF CATALYST
1. A catalyst remains unchanged chemically at the end of the reaction.
2. A small amount of catalyst is sufficient to change rate of reaction.
3. A catalyst has no influence on equilibrium point.
4. It cannot initiate a reaction.
5. It has a selective action.
6. Efficiency of a catalyst depends upon its physical state.

## 3. NANOMATERIAL IN CATALYTIC CONCEPTS
Both organic and inorganic carbons play very important role in nanomaterial catalytic concept. The physical and chemical properties of carbon materials, such as their porosity and surface chemistry make them most useable for application in many catalytic processes; they are generally used as supports for catalysts in heterogeneous catalytic processes. Many carbon materials have been studied of which activated carbon (AC) and carbon black (CB) are commonly used carbon supports. Activated carbons also called as activated charcoal comprises a group of substance having high porous internal surface area and hence absorbing chemical reactants from liquid and gases state. The adsorption is due to Vander Waal's forces. Whereas Carbon blacks, a very pure form of soot is that materials that have spherical carbon particles of average aggregate size is in the range of100-800 nm or above. High porous nature and larger surface area of activated carbon and carbon black catalysts favor the dispersion of active phase on support and hence increases its resistance tosintering at high metal loadings.A carbon material are generally water hating substances i.e. hydrophobic in nature and shows low affinity towards polar solvent such as water and has high affinity towards solvents such as acetone. Other advantages of carbon materials are as follows: a) metals on the support can be easily reduced, b) structures of carbon are resistant to acids and bases, c)structure is stable at high temperatures (above 1023K under inert atmosphere), d) porous carbon materials can be prepared in different physical forms as granules, cloth, fibers, pellets, etc. e) cost of carbon supports is usually lower than that of other supports such as alumina and silica.

## 4. CARBON MATERIALS IN THE ROLE OF CATALYSTS
The reactions catalyzed by carbon materials are classified in following groups (along with examples):

Oxidation reduction:

$2\ SO_2 + O_2$----------------->$2\ SO_3$

$2H_2S + O_2$------------------> $S_2 + 2H_2O$

Hydrogenation-dehydrogenation:

$RX + H_2$-------------------->$RH + HX$ (X = Cl, Br)

HCOOH-------------------->$CO_2 + H_2$

Combination with halogens:

$H_2 + Br_2$------------------->2HBr

$CO + Cl_2$-------------------> $COCl_2$ (phosgene)

Decomposition:

$2H_2O_2$-------------------->$2H_2O + O_2$

$CH_4$ -----------------------> $C + 2H_2$

Dehydration:

HCOOH-------------------> H2O + CO

Isomerization:

$3C_2H_2$---------------------> $C_6H_6$

Polymerization:

α-Olefins -----------------> poly (α-olefins)

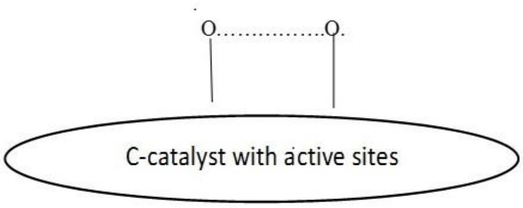
### 4.1 Mechanism of Catalytic Action

For explaining the mechanism let us consider the first reaction of oxidation-reduction i.e.

$2SO_2 + O_2$--------------->$2SO_3$

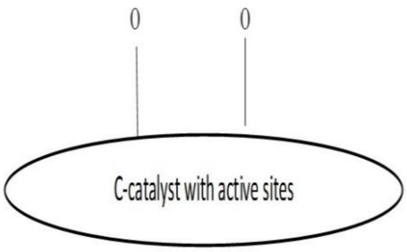
Step I:

Adsorption of oxygen molecules on the catalyst surface due to residual valence bonds of Carbon atom



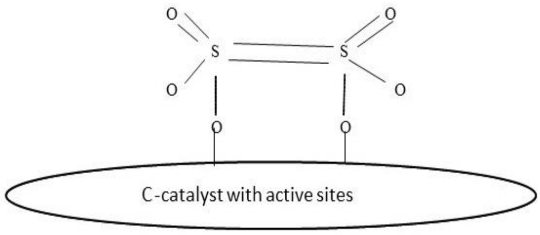

Step II:

Since the bond length of O-----O bond, is lesser than the bond length of C------C bond, the O-------O bond is stretched, weakened and hence broken into atoms which are held to thecatalyst surface by chemical bonds.



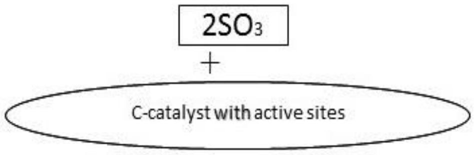

Step III:

The chemically adsorbed O atoms are attached to Sulphur dioxide molecules by partial chemical bonds, thus forming an unstable activated complex.




Step IV:

The unstable activated complex is decomposed to yield the product (Sulphur trioxide) and the catalyst surface is released for a fresh cycle of the above steps.




Other carbon substances which also have a wide variety of applications as catalyst on nanoscale are as follows:

Carbon nanotubes and nanofibers:- These are produced by the catalytic decomposition of certain hydrocarbons. By careful manipulation of various parameters we can be able to control its crystalline order. They can be either single-walled (SWCNTs) (diameter close to 1nm) or multi-walled (MWCNTs) (distance between graphene layers approx. $3.4A^o$). When wrapped SWCNTs form a one atom thick layer of graphite into a seamless cylinder whereas MWCNTs constitute to be multiple rolled layers or concrete tubes of graphene and hence the nanoscale tubular morphology of CNTs offer a unique combination of low electrical resistivity and high porosity. It also offers the advantage of doping giving rise to P-doping and N-doping which also have high catalytic properties.

Propane----$^{\text{CNTs (773K)}}$ -------------------> Propene

Butane------$^{\text{P-Doped CNTs (723K)}}$ -----------> Butene

Propane ---$^{\text{N-Doped CNTs (673K)}}$ ------------>Propene

Graphene and Few-layer Graphene (FLG):- It provides a two dimensional model of catalytic support of $sp^2$ hybridized carbon atoms, the parent material of CNTs. Inculcation of catalyst particles onto FLG can provide a great variety in carrying out catalytic processes and is a new upcoming of the carbon – supported catalyst family.

Iso-Butane ----$^{\text{FLG (673K)}}$ -----------------> Iso-Butene

## 5. APPLICATIONS OF NANOCATALYSTS

Catalysts of nano size are used in several chemical processes which are useful for human beings. These applications of nanocatalyst are reported within last few years

1) In water purification (Ag, $Al_2O_3$, C catalyst)
2) In bio-diesel production ( KF, CaO catalyst)

3) In fuel cell application (Pt catalyst)
4) In drug delivery (CNTs catalyst)
5) In solid rocket propellents (Al catalyst)
6) $TiO_2$ in energy application ($TiO_2$ catalyst)
7) In photochemical activity of $TiO_2$ ($TiO_2$ catalyst)
8) In Thin film solar cell (CdS and $TiO_2$ catalyst)
9) In waste water treatment (Pd catalyst)
10) In environment protection (Fe-Co mixed oxide nanocatalyst)
11) In preparation of fuels ( Ni catalyst supported on nano-particles of $ZrO_2$)
12) In oxidation of alcohol (Pt-Pd/C catalyst)

# 6. CONCLUSION

Explosive growth has been undergone in the field of nanocatalysis i.e. nanoparticles to catalyze reactions in homogeneous and heterogeneous catalysis during the past decade. Compared to bulk material nanoparticles have a large surface to volume ratio and hence are attracted to be used as catalysts. Thousands of chemical reactions are daily accelerated and boosted by catalyst which forms the basis of worldwide spread chemical industry. The ability tocontrol materials on nanoscale will ensure a rational and cost efficient development of more capable catalysts for chemical reactions. Research in nanotechnology and nanoscience is expected to open a new era in environmental protective technologies.

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