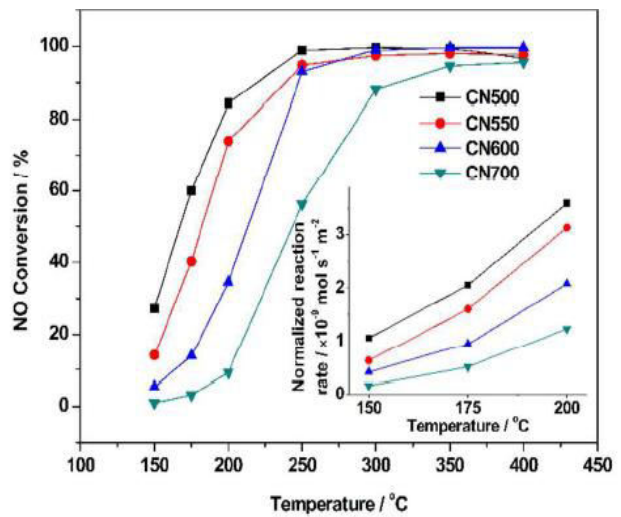


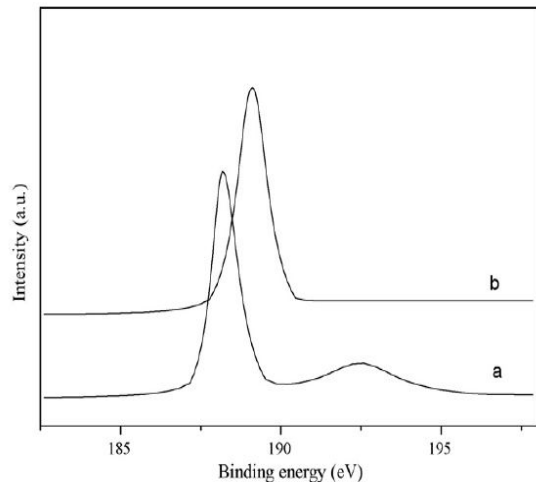
There are different species responsible for catalysis other than input components. Here I have chosen a few of them from literature and explained with the example of NO_x reduction. In the combustion of fossil fuels, this vital air pollutant is generated from motor vehicles and industrial operations. For catalysis of reduction of NO_x, vanadium free catalysis has been developed and measured its activity at different calcination.

- Specific Surface Area**- As we know that the surface area is an essential parameter for the catalysis in solid-state reactions, which is also known as heterogeneous reaction (Reactants are in different phases). BET method can be used to calculate the specific surface area(m²/gram) of catalyst and thin powder. In this method, the specific surface area of solid is measured by suspending an analyte in inert and measuring the absorption of gas molecules in the surface or porous solid material. It can be understood by the simple example of NO_x reduction. For that vanadium free catalyst has been developed using Ce-Nb mixed oxides and calcined at 500°C,550°C,600°C and 700°C for 5hrs and these catalysts are represented as CN500, CN550, CN600, and CN700. Here, it can be seen that at high temperatures (300°C to 450°C) every catalyst has the same conversion efficiency or activity. However, there can be much difference in conversion observed in the temperature range of 150°C to 300°C. The catalyst which calcined at 500°C has the best conversion efficiency. Here it can be concluded that the higher the calcination temperature, reduces the catalytic activity because it changes the specific surface area which is measured by BET analysis.



- **Material properties (Crystalline and Amorphous)** – Amorphous materials are

always used as a catalyst and also gives good catalytic activity but the researchers have always focused on the supporting material and secondary metal which can enhance the activity. However, crystallization is the important property of a material. It can be seen while changing the material property from amorphous to



crystallization through glass transition temperature that side reactions occurred. Activation energy is also affected due to Crystallization. Nevertheless, crystallinity could be achievable after a novel low-temperature ethanol treatment that replaced water with ethanol. Here it can be understood by Amorphous and crystallized Co-B particles as a catalyst for CMA hydrogenation. While crystallizing the material, there is an enormous change in specific surface area which affects the catalytic activity. Hence, it can be deduced that crystallinity and specific surface area are correlated and depend on each other. In these XPS results, there is no side reaction in crystallization. In an amorphous state, there are two peaks found one is for elemental state and another one is for oxidation state but at crystallization state, there is one peak found.

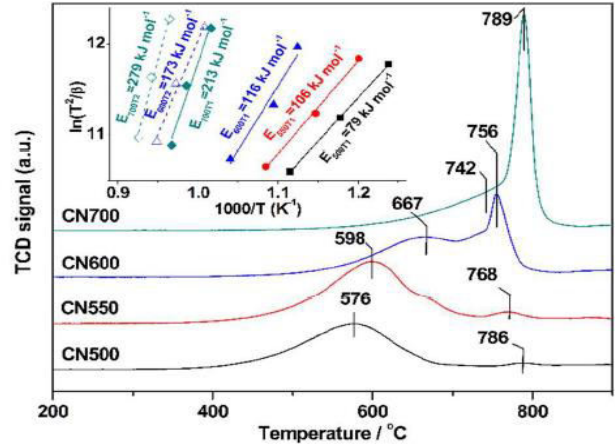
- **Concentration of surface elements** – The concentration of elements present on the surface has significant importance on catalytic activity. It can be determined by the XPS method. It can be observed that during calcination the concentration of niobium is increased because niobium oxides cover all the surface of the catalyst. The result of XPS is tabulated in the molar ratio of niobium and cerium and also specific surface area. As the calcination

Sample	$S_{BET}(m^2/gram)$	Nb/Ce
CN500	123	1.50
CN550	108	1.93
CN600	62	2.21
CN700	26	2.25

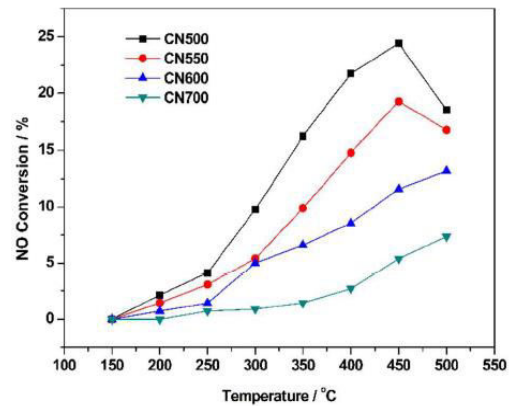
temperature increases niobium concentration increases and also the reduction of specific surface area decreases. Hence, it can be concluded that the ratio of Nb/Ce is optimized at which maximum surface area will be effective.

• **Reduction of surface active oxygen species**

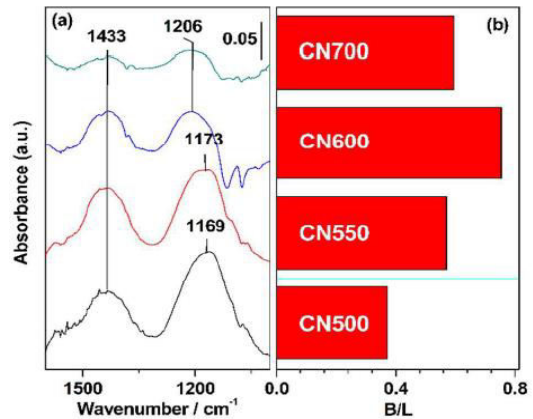
- The H₂ TPR (Temperature programmed reduction) is used to discover the redox property of material which plays a very important role in catalysis. Here it is visible in the figure that CN500 and CN550 having large peaks before 700°C and after the lower peak. However, the same peaks for CN600 and CN700 are overlapped into the leading peak. The first peak for all four samples is denoted as the reduction of surface-active oxygen and it is in order of CN500 to CN700 in ascending. The second peak is denoting a reduction of bulk oxygen species. Also, there is the activation energy of the catalyst which is following the same order as the reduction peak follows but the activation



energy for the first peak of CN700 is lesser than the activation energy of the second peak of CN600. Hence it deduced that oxygen species CN700 is not as active as in CS600. It can be inferred from the shift in the first reduction peak as temperature increases and enhancement in activation energy that the activity of surface oxygen is so much reduced when it calcined at higher temperature thus declining of NO oxidation ability.



- Ratio of Bronsted acid site to Lewis Acid sites(B/L)** – The ratio of Bronsted acid site to Lewis acid site is represented as B/L ratio which is the indicator of the distribution of surface acid sites on the catalyst surface. *In situ DRIFTS* is one of the methods to characterize the surface of the catalyst using NH_3 adsorption. In this figure NH_3 adsorption at 100°C on Ce-Nb oxide catalyst with different calcination temperatures. In these spectra, the second peak which is at 1169, 1173 and 1206 cm^{-1} represented the Lewis acid site and the first peak represents the Bronsted acid site. However, the B/L ratio is increasing from CN500 < CN550 < CN600 but CN700 is less than that CN600 is because of the formation of bulk Niobium oxide on CN700.



Thus it can be seen that how just altering the physical parameters of the catalysis process, these changes occur in the catalyst which can enhance or reduce the activity of catalysts. Specific surface area is playing in an important role which is related to almost all other parameters during alteration. By balancing the specific surface area, material property, acid sites on the catalyst surface, and surface active oxygen species can be controlling factor in the field of catalysis.