Q1: What are the active site of catalyst?

A1: Active site is a point on the catalyst surface that can form strong chemical bonds with an adsorbed atom/molecule. These sites are unsaturated atoms in the solid resulting from:
Surface irregularities, dislocations ,edges of crystals and cracks along grain boundaries

Q2: What is dispersion of catalyst?

A2: Dispersion is the fraction of atoms of a material exposed to the surface. In general $D = N_S/N_T$ where D is the dispersion, N_S is the number of surface atoms and N_T is the total number of atoms of the material. Dispersion is an important concept in heterogeneous catalysis, since only atoms that are exposed to the surface are able to play a role in catalytic surface reactions. Dispersion increases with decreasing crystallite size and approaches unity at a crystallite diameter of about 1 nm.

Q3:What is Sabatier's principle?

A3: This states that there must be an optimum of the rate of a catalytic reaction as a function of the heat of adsorption. If the adsorption is too weak the catalyst has little effect, and will, for example, be unable to dissociate a bond. If the interaction is too strong, the adsorbates will be unable to desorb from the surface. Both
extremes result in small rates of reaction.

Q4: What is Density Functional Theory–Generalized Gradient Approximation (DFT–GGA).

A4: Generalized Gradient Approximation (DFT–GGA) depends on addition of gradient of the electron density. DFT–GGA calculations are very useful for investigating plausible reaction pathways of various molecules on surfaces. The method provides detailed information on the bonding geometry, on bond energies as well on activation barriers, and transition states which are otherwise not accessible. Typical accuracies in such

numbers amount to a few tenths of an eV, making the method particularly useful to investigate trends.