

Surface Hypothesis of Adsorption with Respect to Rare Earth Metals

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Abstract: *Understanding surface chemistry is required to know various phenomena involved at surface level. To understand absorption it involves basically the heterogeneous catalysis to trigger the reaction at the surface. First principle theory and Ab initio modeling set their footprint in the field of catalysis by explaining shrodinger wave equation. So, is Density Field Theory characterizing and customizing using it with respect to the density. But due to its limitation it can laid major dependence on First principle theory to explain the surface phenomena in detail.*

Keywords: Adsorption, First principal theory, Ab initio modeling and Density field theory

1. Introduction

"A catalyst is one which can increase the rate of chemical reaction". Lets give insight of it saying, if K is the reaction constant and is low then even if thermodynamically allowed it will take long time to complete but use of catalyst increase the rate of reaction. In this paradigm heterogeneous catalyst is effectively working on the high surface area of the porous oxides. Heterogeneous catalysis is involved in chemical reaction including bulk mass transfer and the diffusion. Catalytic reaction like these can be modeled by a Arrhenius equation. Reaction progress can be as per the reaction kinetics or the thermodynamic equilibrium attained in the reaction. On the other hand if the reaction reaches equilibrium then progress is thermodynamically impossible.

Thus, Surface chemistry involves the interaction of solid state and liquid or gases phase which is amalgamation of condensed matter physics and chemistry.

Major understanding at the surface chemistry involves electrochemistry and part of the heterogeneous catalysis. Heterogeneous catalyst is alone has been contributing 20% of the major production in the world industry [1]. The key is to provide an efficient mechanism for the transformation of one form of energy to another by suitable catalyst to fulfill the aim of sustainable growth as it is limited by efficient and economically viable kind of catalyst [2 - 3]. The description of the chemical bond between the surface and the molecule sets the fundamental basis of the understanding surface chemical reactivity and catalysis process through many theories. This in turn requires great amount of understanding for the absorption of atoms and molecules at the surface level [4, 5, 6, 7, 8]. Number of theories has been developed to understand this surface chemistry. Out of this we start with the first principle theory, as the name suggest it is basically the first principle derived for the surface chemistry reactions.

2. Literature Survey

First Principle Electronic Structure Calculation for Catalytic Design:

First principle theory brings strong coherence and correlation of catalytic activity and valance electron structures. It provides information on possible combination of elements. First principle corresponds well with the calculation of the electronic structure into metals and alloys which bring strong correlation between the catalytic activities and the valance electron structures. It provides correlation on possible combination of elements. First principle theory is more used in a print primitive manner.

In the series of generation of the catalytic theories **Ab initio model** means also from "first principle theory" extended and defines the work of different reaction mechanism which can get fit in extracting the data. Here quantum calculations for Schrodinger wave function type parameter is required to be fit in the elementary process to define the rate constant for the reaction [9]. Sabbe et. al [10] defined the first principle of micro kinetics considering both theories, which is required because every atom counts having different structure and has insufficient characterization. This theory aims to define lattice structure and includes the thermo chemical calculations like absorption, lateral interactions, Desorption, enthalpy etc. To bring the different connection between different thermodynamic parameters like pressure and temperature gap, Ab initio thermodynamics theory will be there to provide the relation between the micro and the macroscopic parameter [11].

In 1935 it was proposed by the researchers few important exemptions in context to previously called previous rate theory called transition state theory for activated complex form in the compounds on the potential energy surface while attaining the equilibrium [12 - 13]. Many more theories involved for the transition state formation and to determine the bond length [14 - 15]. Due to their limited availability of chemical interaction involving catalytic parameters of rare earth metals and Aqueous media makes up a essential area of research. Bailey et. al. [16] attempted to put forward various thermodynamic properties between within aqueous media. Depending on the nature of the different rare metal

earth matter involves parameters like solubility and the base behavior, potential of the hydrogen etc research will select few elements out of them a majorly outlines its approach. Effect of temperature and pressure are also point of study and concern in these equilibrium reaction [17]. Thus, kinetics and the mechanism of the rare earth metals with respect to its catalytic potential in Aqueous media includes the types of the models like Langmuir and Freundlich adsorption [18].

Density functional theory (DFT)

Density function theory is a critical tool for catalyst and its reaction. The d band model is proved to be good in understanding the bond formation and trends in the transition metal [19 - 20]. The correlation between the interaction energy and the d band Centre has been found in agreement with adsorption and the transition state energy. The kinetics of a catalytic reaction can well understand by density functional theory calculation. But we will focus on the trends in the reactivity that causes variation in kinetic from one surface to the next. Kinetics is basically the summation of reaction and activation energy. For each new catalytic structure and composition a new micro kinetic model is developed for the evaluation of the catalytic structure. Understanding the reactivity it trends to single out the major parameters for considering the catalytic activity. For tailoring of surfaces using Density Function Theory is important. Using Density Function Theory error while calculating the relation could be minimized due to the volcano relationship between the reaction and the transition energies at the surface. The volcano relationship is the major step towards the identification of heterogeneous catalyst, as it is the precursor for the identification and the Solemnization of best catalytic material.

Problem identification and Results

DFT works well for the transition metals but it works worst for the classes of potential catalyst [21, 22, 23, 24, 25]. Even though some progress has been made towards understanding the electro catalytic process through DFT, but improvements are required under DFT as its scope is limited and it cannot treat electronic band gap and excited Electronics states.

For higher accuracy DFT can be a breather but not for the ones when computational intervention is required. Density Field Theory and the d band model has wide application for oxide as it is the bond formation and interaction of adsorbents valance states of s and d orbital state at the surface of the transition metals. The coupling gives rise to the broadening of the adsorption states which is due to the bonding and anti - bonding states between the Valance s and d states. Antibonding state broadly classified energy at the fermi level which defines bond length in DFT theory and d state describe the anti - bonding state. Fermi level is the first indicator of bond strength. So higher is the d anti bonding higher chances of stronger bond. But it limits the fermi level to d band as each metal system compensates on moving up and down in energy which varies with the coordination number. Thus, DFT simulation using Schrödinger's material science is a tool for analysis optimization and discovery. But we need enhanced activity in selectivity of catalyst in this context. All the DFT calculations are limited to spin polarized, considering difficulty with DFT to represent d and

f states with regard to rare earth metal. We implemented DFT plus other theories to approach all DFT calculations work for temperature limited at the 0°K. But ideally real materials are full of defects and impurities so is more treatable with wave function model. Defects and doped material structure and composition which depend on the preparation of the impurities and also the types of adsorbents and it will in turn influence the surface chemistry so needs to be considered also in totality. In the series of the surface generation theories, this is the problem with DFT theory.

3. Conclusion and Future Perspective

First principle theory best describes when it comes to explain the thermodynamics involved at the surface. It is used more in primitive manner and had no restriction with any specific temperature whereas metal separation and adsorption involves the current phenomena pretty well and leaves scope for the further advancement in the same field.

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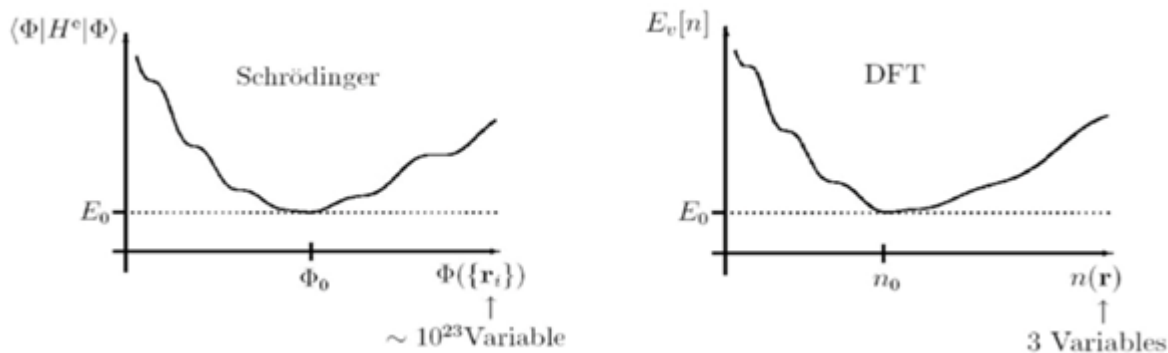


Figure 1