

Review of Emerging Trends in Surface Chemistry

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ABSTRACT

Surface chemistry is a fundamental and radical science that forms the basis of modern materials and technologies. On a molecular level, it controls the behavior of matter because it determines adhesion, wetting, catalysis, and the energy conversion processes that are the basis of innovations in medicine, renewable energy, environmental protection, and ordinary materials. Understanding of surface behaviour also helps the scientists to regulate reactivity, synthesize functional interfaces and develop materials that react best with their surroundings. The review follows the historical development of surface chemistry focusing on the pre-history of the field, current advances, and future developments. Theoretical foundations, e.g., adsorption isotherm of Langmuir and surface energy equation of Gibbs, laid the theoretical basis of explaining interfacial events and adsorption equilibria. Modern directions include nanostructured and biofunctional surfaces, stimuli-responsive interfaces, and environmental systems such as dispersion of oil-spills, control of pollution and purification of wastewater. Surface chemistry is being disrupted by the combination of artificial intelligence, machine learning, and the use of computational modelling to predictively design materials with customized interfacial characteristics. The directions of future research include sustainable and green surface chemistry, in particular bio-based surfactants, renewable nanomaterials and multifunctional hybrid systems to biomedical, catalytic and energy applications. Finally, advances in surface chemistry do not just stop in the laboratory environment; they offer cleaner water, more efficient energy storage, safe materials, and an improved quality of life, which has further supported its core contribution to more sustainable and human-centered technological future.

KEYWORDS: Artificial intelligence, Environmental remediation, Hybrid materials. Nanostructured surfaces, Smart materials, Surface chemistry.

1. INTRODUCTION

Surface chemistry is an interdisciplinary field of chemistry, which studies chemical reactions at the surface of solid materials. The field requires the study of adsorption, migration, assembly, activation, reaction, and desorption processes of atoms and molecules at the surface.¹ Surface chemistry has had a significant impact on numerous technologies due to the fundamental formation of surface chemistry. In the early days related to Langmuir and Ertl, the improvement of the performance of incandescent lamps was viewed as a key technological driving force, which triggered the intensive research of tungsten filament chemistry and the dynamics of molecules adsorbed onto and reacting with surfaces of transition metals; these concepts form the basis of heterogeneous catalysis.² The semiconductor surfaces did grow in popularity in the 1960s, thereby further enlightening the influence of the surface structural features in catalytic and semiconductor sciences. Surface chemistry has long been associated with a significant fraction of the world GDP over many years, and the wide range of applications with high impact has been driving the development of surface chemistry, including electronics, petrochemicals, fixing nitrogen on fertilisers, and automotive catalyst technology. Other upcoming fields are photovoltaics and a wide range of energy conversion technologies.²

Contemporary surface chemistry is based on a molecular level concept and exact control of surface based chemical reactions. Numerous surface-science methods have been developed in the past decades, and a large body of knowledge on surface chemistry has been accumulated.^{3,4,5} This is a cumulative knowledge that forms the basis of many industrial technologies which manufacture chemicals, fuels, semiconductor devices and biomedical apparatus. Advancement in technology, in turn, contributes towards the further development of surface-characterization methods of increased space, time, and energy.⁶ Recent publications have shown that operando and spatially resolved probing technology can be used to apply laboratory results to operational and that interface-specific

structural and dynamical markers can be used to correlate the molecular orientation with functional output with the aid of vibrational nonlinear optical methods that include the sum -frequency generation.^{7,8} At the same time, operando X-ray and ambient-pressure photoelectron spectroscopies clarify the evolution of chemical states on catalytic surfaces under conditions that are realistic thus enhancing mechanistic understanding of reactions of relevance in industry.⁹

Surface chemistry is a crucial part of various scientific and industrial aspects, which disposes of material interactions on both molecular and macroscopic levels. Since the initial developments of adsorption and catalysis were first explained, the field has developed significantly to its current uses in nanotechnology, storing energy and environmental sustainability. This review discusses the history, current advances and future trends of surface chemistry. Surface chemistry in the present age is the source of innovation in nanostructured surfaces, self-assembled monolayers, and smart surfaces that have adjustable properties. It is noted that these materials find more and more applications in different fields such as energy conversion, environmental remediation, biomedical engineering, and industrial manufacturing.¹⁰ In addition, the design and optimization of functional surfaces are also being turned by integrating artificial intelligence and computational.^{11,12}

In the future, surface chemistry is expected to play a major role in the development of sustainable materials with particular applications in biodegradable surfactants, environmental friendlier coatings and multifunctional hybrid surfaces. This is a review that provides an in-depth discussion of the recent trends in surface chemistry covering past successes, present developments, and future directions of research.

2. HISTORICAL DEVELOPMENT OF SURFACE CHEMISTRY

The area of surface chemistry started with heterogeneous catalysis pioneered by Paul Sabatier on hydrogenation and Fritz Haber on the Haber process. Irving Langmuir was also one of the founders of this field, and the scientific journal on surface science, Langmuir, bears his name. The Langmuir absorption equation is used to model monolayer adsorption where all surface adsorption sites have the same affinity for the adsorbing species and do not interact with each other.¹³

Gerhard Ertl in 1974 described for the first time the adsorption of hydrogen on a palladium surface using a novel technique called LEED. Similar studies with platinum, nickel, and iron followed. Most recent developments in surface sciences include the 2007 Nobel prize of Chemistry winner Gerhard Ertl's advancements in surface chemistry, specifically his investigation of the interaction between carbon monoxide molecules and platinum surfaces.¹⁴

The foundations of surface chemistry were laid by early studies on adsorption, catalysis and surface interactions. Langmuir's adsorption isotherm (1918) was a breakthrough in understanding gas adsorption on solid surfaces at different concentrations. While Langmuir's work laid the foundation for heterogeneous catalysis and surface modification, Freundlich's empirical model further contributed to the understanding of multilayer adsorption on heterogeneous surfaces.^{15,16}

Later, the development of scanning probe microscopy (SPM) and X-ray photoelectron spectroscopy (XPS) provided detailed insights into surface structures at the atomic level.¹⁷

Early studies in surface chemistry were centered on adsorption, catalysis, and surface interactions. Langmuir¹⁶ introduced the adsorption isotherm, which described how molecules adhere to surfaces at different concentrations. The development of the Gibbs adsorption equation explained how surfactants lower surface tension by accumulating at interfaces, influencing emulsification and wetting processes.¹⁸ In the mid-20th century, advancements in surface spectroscopy techniques, such as X-ray photoelectron spectroscopy (XPS) and Auger electron spectroscopy (AES), enabled atomic-scale surface analysis, improving the characterization of catalytic and adsorption processes.¹⁷

2.1 Adsorption Isotherm

A variety of isotherms have been applied in adsorption systems, such as the Langmuir model, linear model, the Freundlich model, the Sips model, the Temkin model, and the Brunauer, Emmett, and Teller (BET) model.¹⁹

2.2 Langmuir Isotherm

The Langmuir isotherm was initially developed for gas–solid interaction but is also used for various adsorbents. It is an empirical model based on kinetic principles; that is, the surface rates of adsorption and desorption are equal with zero accumulation at equilibrium conditions. Based on the following assumptions, (a) monolayer adsorption, (b) homogeneous sites, (c) constant adsorption energy, and (d) no lateral interaction between the adsorbed molecules, the Langmuir isotherm can be written as

$$q_e = q_o K_L C_e / 1 + K_L C_e \dots\dots\dots(1)$$

where q_o is the maximum amount of adsorbed surfactant in and K_L is the Langmuir constant in. The linearized version of the equation is

$$C_e/q_e = 1/K_L q_o + C_e/q_o \dots\dots\dots(2)$$

A plot between C_e/q_e versus C_e will generate a straight line with a slope of $1/q_o$ and an intercept equals to $1/K_L q_o$.

The monolayer assumption requires identical adsorption sites, and only one molecule can be adsorbed at each site. There is no more adsorption in a site once a surfactant molecule has occupied it.

2.3 Freundlich Isotherm

Unlike the Langmuir isotherm, this empirical model can be used for multilayer adsorption on heterogeneous sites. It assumes that the adsorption heat distribution and affinities toward the heterogeneous surface are non uniform. The mathematical model can be shown as

$$q_e = b C_e^{1/n}$$

where b is the adsorption capacity and $1/n$ is the adsorption intensity or surface heterogeneity. When $0 < 1/n < 1$, adsorption is considered favorable. Unfavorable adsorption occurs when $1/n > 1$ and is irreversible at $1/n = 1$.

The linearized form can be written as

$$\ln q_e = \ln b + \frac{1}{n} \ln C_e$$

A plot of $\ln q_e$ versus $\ln C_e$ produces a straight line with a slope = $1/n$ and intercept = $\ln b$.

The linearized form is easy and straightforward. On the other hand, the linearization process generates propagating errors, which results in erroneous predictions of parameters. Therefore, the use of nonlinear regression to solve the nonlinear Freundlich model is recommended for the calculation of the model parameters.

The Freundlich isotherm describes multilayer adsorption and assumes exponential decay in the energy distribution of adsorbed sites. However, it is not valid for a large range of adsorption data.²⁰

2.4 Applications of adsorption isotherms

There are several possible applications of adsorption isotherms. The following points introduce short key highlights on applications of adsorption isotherms:

To compute the capacity and percentage removal of adsorbates from a certain media or environment.

To acquire the greatest adsorbent absorption and affinity between adsorbent and adsorbate, Langmuir parameters can be applied.

Freundlich parameters can be used to obtain adsorption capacity of adsorbents.²¹

2.5 Surface chemistry in adsorption process

Adsorption process is a surface phenomenon in which adsorbates transfer onto adsorbents. Over the past decades, adsorption technology has been widely applied for the water and wastewater treatment because it is low-cost, efficient, simple, and environmentally friendly

Adsorption is the adhesion of an adsorbate such as a fluid, liquid, or gas, by creating a thin layer or film on the surface of an adsorbent whether it is a solid or liquid as shown on figure 1.

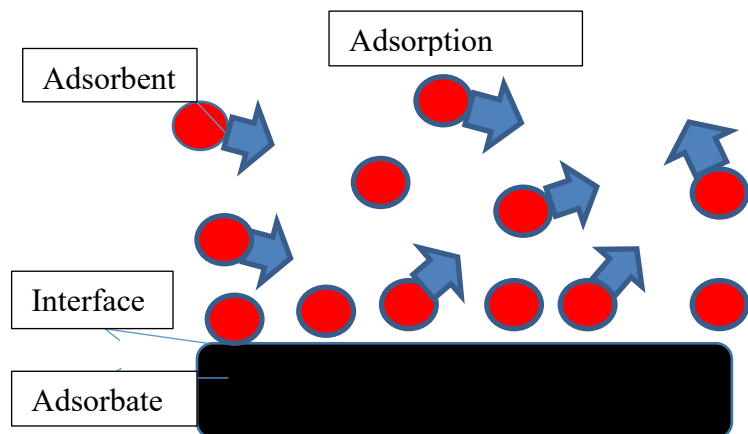


Figure 1 Adsorption on adsorbent

The bonding between adsorbate and adsorbent could be physical or chemical bonding as shown in figure 2. The adsorption mechanisms include chemical adsorption corresponding to the formation of chemical bonds, physical adsorption related to the van der Waals force, and the ion exchange. The knowledge of adsorption mechanisms is of great importance to design the adsorbents and the adsorption systems. The chemical bonding provides stronger bonding than physical bonding, layers. Adsorbate can be separated from the adsorbent and the process is called desorption. There are some factors influencing the adsorption process, but, at the basic level, the most widely studied is the influence of temperature and could be assumed as a monolayer. The adsorption process is usually studied at a given temperature and recognized as an adsorption isotherm.²²

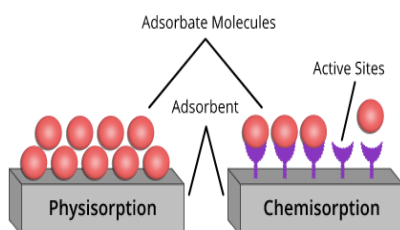


Figure 2 Physisorption and Chemisorption on adsorbent

3. PRESENT TRENDS IN SURFACE CHEMISTRY

3.1. Nanostructured and Functionalized Surfaces

Recent advances in nanotechnology have led to the development of nanostructured surfaces with tunable properties. Graphene-based coatings, metal-organic frameworks (MOFs), and self-assembled monolayers (SAMs) have shown promise in applications such as catalysis, biomedical engineering, and energy storage.²³ Studies by Zhang et al.²⁴ highlight the fabrication of bioinspired

superhydrophobic surfaces, mimicking the lotus leaf effect for antifouling and self-cleaning applications.

3.2. Surface Chemistry in Environmental Remediation

Surface chemistry is increasingly applied in oil spill remediation, wastewater treatment, and pollutant adsorption. Wang et al.²⁵ demonstrated that engineered surfaces with hydrophobic/hydrophilic balance enhance oil-water separation efficiency. Additionally, Jiang et al.²⁶ investigated surface-modified bioadsorbents for heavy metal and fluoride removal from contaminated water sources. The use of surfactant-functionalized nanomaterials has further improved adsorption capacity and selectivity for toxic pollutants.

3.3. Smart and Responsive Surfaces

Advancements in stimuli-responsive materials have enabled the development of smart surfaces that change their properties based on external triggers such as temperature, pH, or light.²⁷ Photo switchable molecular receptors have been explored for controlled adsorption and release of pollutants, offering potential applications in chemical sensing, self-healing coatings and drug delivery.²⁸

3.4. Surface Chemistry in Energy Applications

Surface chemistry modifications play a crucial role in improving the efficiency of electrocatalysts for hydrogen production, fuel cells, and lithium-ion batteries. Zhao et al.²⁹ reviewed advancements in surface-engineered electrode materials that enhance charge transport and stability in energy storage systems. Similarly, surface-functionalized perovskite materials have shown promising efficiency in boosting solar cell.³⁰

4. FUTURE PROSPECTS IN SURFACE CHEMISTRY

4.1. Sustainable and Green Surface Chemistry

As sustainability concerns grow, green chemistry approaches in surface engineering are gaining traction. The shift toward eco-friendly and biodegradable surfactants is gaining momentum, with researchers exploring plant-based and sugar-derived surfactants as sustainable alternatives to synthetic surfactants.³¹ Bio-based coatings are also being developed for corrosion protection and antimicrobial applications.³²

4.2. Advanced Computational Surface Chemistry

Computational modeling like, Machine learning and other Artificial Intelligence -driven approaches are transforming the way surface chemistry is studied. Computational simulations help predict surface interactions, optimize coatings, and design self-healing materials.³² The application of density functional theory (DFT) has further improved the understanding of molecular-level surface modifications.²⁹

4.3. Multifunctional and Hybrid Surface Materials

These are hybrid surfaces that focus on multifunctional hybrid materials, integrating self-cleaning, antibacterial, and conductive properties into a single surface.³⁰ These materials hold promise for applications in biomedical implants, electronic devices, and aerospace coatings.³⁰

5. CONCLUSION

This study highlights the evolution of surface chemistry from classical adsorption theories to advanced functionalized materials. The field has witnessed a shift toward nanotechnology-driven surface

engineering, smart interfaces, and sustainable surface modifications. Future advancements are expected to integrate AI-driven material design and multifunctional hybrid surfaces, addressing critical challenges in environmental sustainability, energy efficiency, and biomedical applications.

CONFLICT OF INTERESTS

The authors declare no conflict of interests.

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