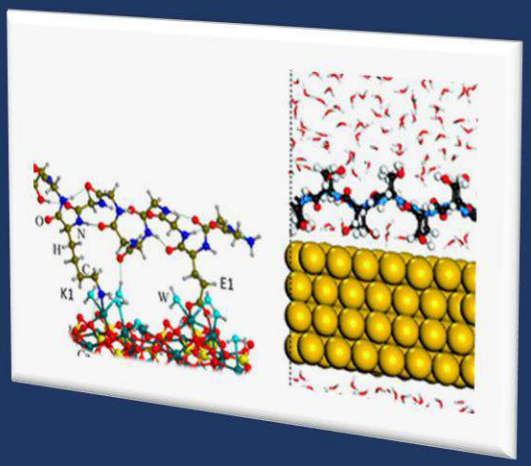
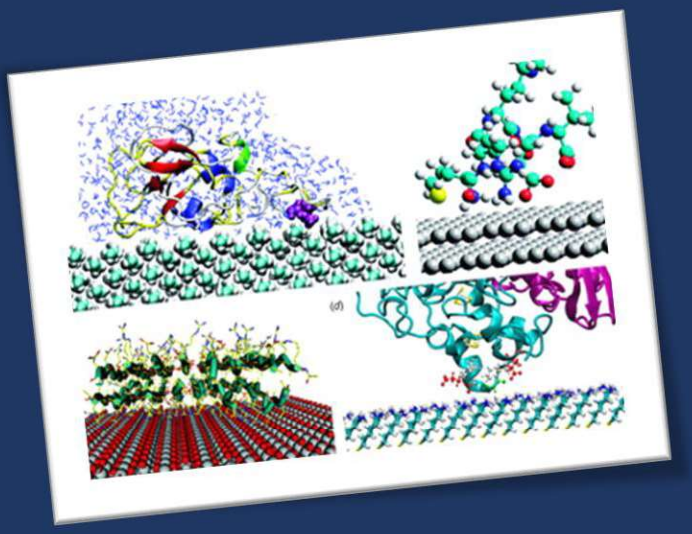
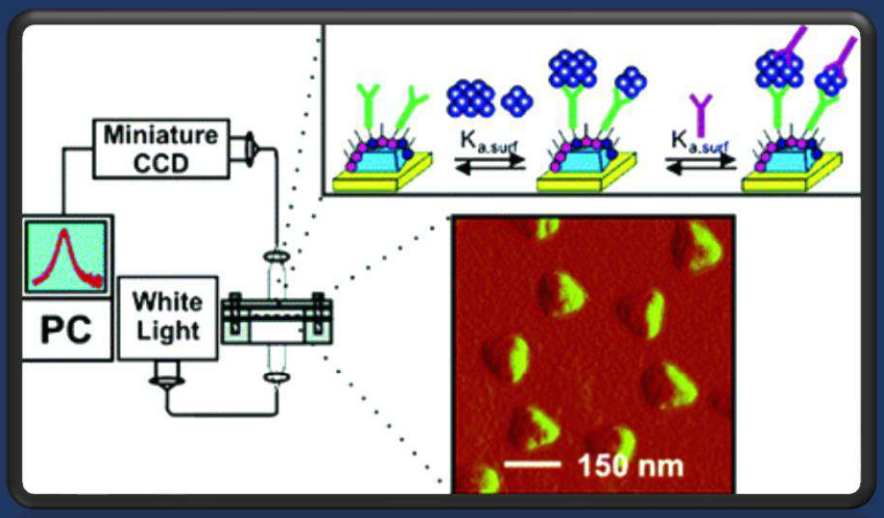
Chapter 6

Summary and Future Prospects







The research conducted in this thesis is characterized by its open-ended nature, offering substantial potential for future explorations into the materials and the properties being studied. Within the scope of this thesis, the calculation of unique properties of novel materials has consistently been carried out through the utilization of Density Functional Theory (DFT) and Classical Molecular Dynamics (MD) simulations. Over recent years, Density Functional Theory (DFT) and Molecular Dynamics (MD) simulations have emerged as pivotal research tools within the field of materials science. This rise in prominence can largely be attributed to significant improvements in computational capabilities, the development of efficient numerical techniques, and the introduction of various novel exchange-correlation functionals. The first two chapters of the thesis offer a thorough introduction to new trends that are being created to reduce the dimensionality of materials in order to gain access to desired unique material characteristics for use in emerging fields such as electronics, optical, and biological applications. We also briefly delved into the realm of two-dimensional materials, encompassing graphene, as well as delving into other low-dimensional carbon structures like carbon nanotubes (CNTs) and fullerenes.

The interaction mechanism of different nucleobases (Adenine (A), Thymine (T), Guanine (G), Cytosine (C) and Uracil (U)) with the C_{24} fullerene (D_{6d} symmetry) and the binding sequence with the C_{24} are explored using dispersion (D3) corrected density functional theory. To evaluate the interaction between the nucleobases with the C_{24} fullerene, we have calculated adsorption energy, NBO analysis, Mulliken charge analysis, density of states, sensing response and recovery time. In our investigation, it has come to our attention that there is a significant and resilient chemical interplay occurring between Adenine and C_{24} fullerene when they are in a gaseous state. This intriguing phenomenon implies a heightened responsiveness during sensing and an extended recuperation period. This intriguing revelation raises the possibility of utilizing C_{24} fullerene as a DNA biosensor, primarily for the purpose of distinguishing adenine from the other constituent DNA nucleobases. On the other hand, when considering Cytosine, Guanine, Thymine, and Uracil, we have observed their adherence to the C_{24} fullerene through a process known as physisorption. However, it's noteworthy that this interaction results in notably shorter recovery periods of only 10^{-14} s seconds and minimal sensing responses. Among the various nucleobases we studied, it is noteworthy that Cytosine and Guanine exhibit the most favorable interaction energies and shorter distances between their constituent atoms when paired with C_{24} fullerene. This finding suggests that the C_{24} fullerene

holds promise as an effective detector for these particular nucleobases. On the other hand, our analysis reveals a relatively weak interaction between thymine and uracil with C_{24}.The electrical and adsorption analysis exhibit that the thymine shows slightly stronger interaction compared to uracil. The solubility of Adenine/C_{24} in water is notably compromised, primarily because its solvation energy falls below that of pure C_{24}. This intriguing difference results in a striking acceleration of both sensing responses and recovery times, particularly for adenine and cytosine. As a result, it becomes increasingly tantalizing to contemplate the application of the C_{24} biosensor as a means of extracting these pivotal nucleobases (Adenine and Cytosine) from aqueous environments. It is crucial to highlight that the interactions involving guanine, thymine, and uracil have undergone a substantial reduction in interaction energy due to the solvent's influence. This intriguing phenomenon translates into decreased reactivity for these nucleobase complexes, leading to significantly shorter recovery times—an aspect that lends itself to their potential utility in detection applications. The paramount conclusion drawn is that C_{24} fullerene emerges as a compelling option for nucleobase sensing, with the exciting prospect of precisely predicting nucleobase sequences within DNA/RNA strands.

Using density functional theory (DFT) and the classical molecular dynamics simulations interaction mechanism between three illicit drug molecules Amphetamine (AMP), Ketamine (KET) and Mercaptopurine (MER) and pristine C_{24} fullerene has been studied. It is essential to underscore our intriguing discovery: within the gaseous realm, AMP and fullerene engage in a remarkably robust interaction, yielding prolonged recovery times and remarkably heightened sensing responses. This fundamentally means that the C_{24} fullerene emerges as a powerful chemical sensor for effectively discerning AMP from a complex mixture of pharmacological compounds. Furthermore, when we delve into the intricate realm of KET and MER interactions with C_{24} fullerene, we uncover a mesmerizing phenomenon—physisorption. This process leads to significantly abbreviated recovery times, as rapid as 10^{-9} and 10^{-10} seconds, and these interactions are accompanied by strikingly discernible sensing responses. It's crucial to underscore the exceptional nature of the interaction energies and interatomic distances that exist between C_{24} and the drugs KET and MER—these characteristics make C_{24} an ideal platform for detecting these specific substances. Furthermore, within a water-based context, the AMP and KET complexes exhibit remarkable reactivity and endurance, thanks to a substantial increase in adsorption energy compared to their behavior in the gaseous phase. It is important to note that the profound impact of pharmaceutical agents like AMP and KET,

significantly expediting both sensing responses and recovery times. A pivotal possibility arises: the extraction of medication compounds such as AMP and KET from a water phase can be realized through the application of C_{24} fullerene. Furthermore, the solvent effect imparts a transformation in the interaction dynamics between MER drug molecules and C_{24}, causing the MER/C_{24} complex to lose some of its reactivity and exhibit a swifter recovery, thus making it an enticing choice for MER detection. Intriguingly, when we delve into the realm of molecular dynamics simulations, the intricate interplay within these complexes unfolds. They not only attain a state of equilibrium but also manifest a remarkable level of stability when subjected to the aqueous environment at room temperature (310K). The RDF plot, a pivotal piece of the puzzle, underlines a crucial point: drug molecules are intricately distributed around C_{24} fullerene in a well-organized manner, maintaining suitable distances—a powerful corroboration of the adsorption mechanisms unveiled by the DFT analysis. Consequently, the synthesis of insights gleaned from both DFT and MD simulations leads to an emphatic conclusion—the versatile C_{24} fullerene emerges as an exceptionally well-suited candidate for not only the efficient removal of AMP and KET drug molecules within water environments but also the precise detection of MER drug molecules at room temperature.

The dispersion corrected density functional theory (DFT-D3) and classical molecular dynamics (MD) simulations assess and comprehend the interaction tendencies of size-variable fullerenes (C_{24}, C_{36}, C_{50}, and C_{70}) towards L-Leucine (LEU), one of the essential amino acids. It is crucial to underscore the significance of our findings—LEU and C_{24} fullerene engage in a remarkably profound interaction within the ethereal domain of the gas phase. This intricate interplay yields a crescendo of heightened sensing responses and an almost enigmatic prolongation of recovery, thereby amplifying the potential of C_{24} fullerene as a biosensor capable of performing a surgical separation of the biomolecule LEU from a complex biological milieu. Yet, the story takes an entrancing turn as we venture into the world of physisorption. Here, the molecular tapestry weaves itself with remarkable brevity, recovering in an astonishing 10^{-10} seconds, leaving behind a trace of discernible sensing response. It's essential to emphasize the profound significance of our findings—the optimal interaction energies and the closely-knit interatomic distances between LEU biomolecules and C_{36}, C_{50}, and C_{70} fullerenes pave the way for envisioning a revolutionary LEU detector built upon fullerenes. What's more, the solvent's influence imparts a transformative impact, elevating the adsorption energies within the LEU/C_{24} and LEU/C_{36} complexes to levels surpassing those seen in the

gaseous phase. This metamorphosis renders them not just responsive but remarkably steadfast in the embrace of a watery environment. Both C_{24} and C_{36} fullerenes exhibit a remarkable ability to greatly enhance sensory responses and recovery times. Consequently, these two fullerenes have the potential to effectively extract the LEU biomolecule from an aqueous environment. On the other hand, the interaction energy between LEU and C_{50}, as well as C_{70} fullerenes, diminishes due to the influence of the solvent. This suggests that the LEU/C_{50} and LEU/C_{70} complexes are less responsive, which might restrict their suitability for LEU detection. It is imperative to underscore the depth of our investigation: through a meticulously conducted classical molecular dynamics simulation, we have uncovered a mesmerizing truth. The LEU/C_{24} and LEU/C_{36} complexes not only reach a state of harmonious equilibrium but also stand as monuments of astonishing stability within the aqueous domain, all under the unassuming gaze of ambient temperature (310K). Moreover, the RDF plots paint a vivid picture—biomolecules are elegantly scattered at discernible distances around the C_{24} and C_{36} fullerenes, serving as compelling validation for the adsorption mechanisms initially hypothesized through our DFT analyses. In conclusion, by synthesizing insights from both DFT and MD simulations, we have determined that C_{24} and C_{36} fullerenes present a compelling prospect as innovative solutions for the creation of advanced biomolecule functionalization and sensor technologies, specifically tailored for high-performance applications in a water-based environment at standard room temperature.

Future Scope

A key focus of this thesis is to attain an in-depth comprehension of carbon nanostructures at the atomic level, while concurrently exploring their affinity for binding, paving the way for potential innovations in the field of biotechnology. In the past few years, low-dimensional carbon materials such as fullerenes, carbon nanotubes etc have gained prominence as intriguing substitutes for graphene-based materials, particularly in the field of bio-applications. These low-dimensional carbon nanostructures provide the opportunity to customize their properties for specific applications. Within the scope of this thesis, our research revolves around the study of bio-conjugation with carbon nanostructures, unravelling their interaction mechanisms, and uncovering their electronic properties.

Several goals have been established as part of our forthcoming expansion strategy. In contrast to graphene-based nanomaterials, where parameters like as production techniques,

size, shape, and working circumstances have a significant role in toxicity and biocompatibility, pristine low-dimensional carbon nanostructures display in vitro and in vivo biocompatibility. We may use molecular dynamics (MD) simulations on large proteins and DNA molecules in combination with carbon nanostructures to evaluate the potential of carbon nanostructures in drug delivery and DNA sequencing. Additionally, there is a glimpse into the potential applications of recently forecasted carbon nanomaterials in both one-dimensional and zero-dimensional formats for the detection and analysis of amino acids and nucleobases, respectively. Furthermore, exploring their responsiveness to harmful drugs and biomolecules holds promise for creating a cleaner and more environmentally friendly ecosystem, making it a compelling and essential area of research. Embracing reduced dimensionalities, nanostructures stand as strong contenders in the realm of electrocatalysis and a myriad of other domains. These diminutive nanostructures have unveiled a plethora of intriguing electrical and magnetic attributes, thanks to an array of innovative functionalization techniques. Nevertheless, a substantial band gap acts as an impediment, preventing them from reaching their maximum capabilities. The modulation of their electronic properties can be achieved through inventive approaches in structural design. Additionally, it is possible to compute the linear responses of the bioconjugate system under consideration. However, it is important to note that such calculations demand a considerable number of computational resources.

"The most incomprehensible thing about the world is that it is comprehensible." - Albert Einstein