Chapter 3

Non-covalent Interactions of Graphene with Polycyclic Aromatic Hydrocarbons*

In this chapter we discuss the interactions of polyaromatic hydrocarbons (PAHs) with graphene and the experimental approaches developed so far to create novel graphene/PAH hybrids and composite systems. The utilization of these systems in electrical, biomedical and polymer-reinforcement applications is described while special emphasis is given to environmental remediation issues.

3.1 Introduction

Graphene, a monolayer of carbon atoms tightly packed into a planar two-dimensional hexagonal lattice surprised the scientific world with its exceptional properties, which differ from those of all the other carbon allotropes discovered so far. Its extraordinary electron mobility, combined with its high thermal and mechanical stability, chemical inertness, large theoretical surface area, elasticity and the possibility to modify electrochemically its electronic structure,[1, 2] place graphene at the top of the list of candidates for the development of new nanomaterials for a plethora of applications including molecular electronics, biosensors, environmental sensors and energy storage nanodevices.[3-7]

On the other hand, polycyclic aromatic hydrocarbons (PAHs) consist of multiple aromatic carbon rings and are considered as small parts of a graphene flake decorated by hydrogen molecules at the edges. They are residues of incomplete combustion of coal, wood, plants, and organic materials as well as
anthropogenic products of fossil fuels (petroleum) and combustion of cars or industry\textsuperscript{8} but can also be produced by direct biosynthesis by microbes and plants. In the atmosphere, PAHs may undergo photolytic and chemical (ozone) transformations. However, most of the material does not degrade quickly in the atmosphere and thus may reside in the environment for extended periods of time\textsuperscript{9}. Finding methods to remove PAHs from the environment as well as for their utilization as nanomaterial building block are two subjects of great scientific interest.


This mini-review attempts to provide a comprehensive and critical overview of the interactions of PAHs with graphene and graphene-based materials. The development of novel graphene/PAHs hybrid and composite systems and their utilization in electrical, biomedical and polymer-reinforcement applications is described. Specific emphasis is given to environmental remediation issues concerning the use of graphene for the effective removal of polycyclic aromatic compounds.

### 3.2 PAHs interactions: Theoretical approaches

PAHs, similarly to graphene, have the tendency to stack together forming 3-D layered aggregates due to non-covalent $\pi$-$\pi$ interactions between the carbon sheets. For this reason PAHs can be viewed as model systems for understanding the $\pi$-$\pi$ interactions between graphene sheets. Theoretical investigations have elucidated the interactions between PAHs and single graphene layers. In fact, density functional theory calculations have been extensively used because they provide precise details concerning the stacking of aromatic rings on the graphene surface at a relatively low cost.\textsuperscript{10-12}
Recently, a van der Waals density functional theory (vdW-DF) approach was applied by Chakarova et al. to describe the interaction between stacked polycyclic aromatic molecules. The same authors also applied vdW-DF to benzene, anthracene, naphthalene and pyrene dimers stacked in sandwich (AA) structure, as well as to the slipped-parallel (AB) naphthalene dimer and infinite graphene layers. The calculated results include non-local dispersion interactions between the dimers and are in accordance with experimental findings.

Moreover, Umadevi and Sastry used DFT calculations to explain the types of interaction of small molecules, metals and ions, such as CO$_2$, H$_2$O, Li$^+$ and Mg$^{2+}$ with various linear and branched polycyclic aromatic hydrocarbons taken as models of truncated graphene sheets (Figure 1). The theoretical results suggest chemisorption of metal atoms or ions on the graphene-like PAH system, while CO$_2$ and H$_2$O are physisorbed on the PAH surface.

![Figure 1](image_url)

**Figure 1**: Schematic representation of graphene-PAHs nanohybrids adsorbing small molecules (CO$_2$, H$_2$O), metals (Mg, Li) and metallic ions (Li$^+$, Mg$^{2+}$). (Reproduced with permission from Ref. [17]).

Yadav and Mishra used gas phase structures to study dimers and trimers of polycyclic aromatic hydrocarbons (PAHs) having zig-zag edges, and continuous electron density and molecular electrostatic potential (MEP) distributions. They tested the reliability of four different functionals of density functional theory on benzene and naphthalene. For dimers the displacements of the monomers along the X-direction and the Y-direction lie between 1.43 and
1.49 Å, while those along the Z-direction equal between 3.36 and 3.41 Å. The centre-of-mass separations between the monomers in all dimers amount to between 3.65 and 3.72 Å. It was found that dimers where the monomers are displaced along the X-axis were more stable by 0.71 and 0.92 kcal/mol than those with displacements along the Y-axis. For trimers two types of stacking of graphene layers were observed, rhombohedral (or ABC) stacking and Bernal (or ABA) stacking. In both dimers and trimers the electron density was not enhanced at all the C–C bonds located at the edges, but most of the C–C bonds where the electron density is enhanced, were located at the edges. The analysis of MEP distributions showed that the enhanced electron density edge effect, found to exist in PAH monomers, persists in PAH dimers and trimers.

3.3 Graphene functionalization by PAHs

Graphene and graphene oxide are widely used as nanofillers in polymers when aiming to improve the thermal, mechanical, and electrical properties of the resulting polymer composites. However, these carbon nanofillers are often poorly dispersed in polymeric matrices, a problem which can be circumvented by different approaches of graphene functionalization. Non-covalent functionalization is preferable in this context since it preserves the structure and associated properties of graphene.

Yang et al.\cite{19} developed a facile method to generate stable graphene suspensions in water by direct exfoliation of graphite in water, based on non-covalent interactions with 1-pyrenesulfonic acid sodium salt (Py-1SO$_3$) (Figure 2). An extensive Raman analysis of the material in suspension revealed that it consists of \ (~70\%) few-graphene layers (<7). For comparison a salt with a different number of sulfonic groups, 1.3.6.8-pyrenetetrasulfonic acid, was also investigated but gave a much lower exfoliation yield, indicating that the exfoliation efficiency depends on the number of sulfonic groups. Apart from being highly effective, this exfoliation method has numerous other advantages:
it is quick, non-destructive, and the used molecules are commercially available and cheap. A promising application of the suspensions thus created is their use as inks for printable tattoo-based electro-chemical sensors, based on the fact that proteins and other biological objects easily graft to pyrene.

![Graphite exfoliation process](image)

**Figure 2:** (A) Schematic of the exfoliation of graphite flakes using 1-pyrenesulfonic acid sodium salt (Py-1SO₃). The process includes different steps (mixing, exfoliation and washing). The washing step is repeated for three times in order to remove the excess Py-1SO₃. (B) Digital picture of a vial containing the resulting graphene-based dispersion. (C) Py-1SO₃ based graphene film prepared by vacuum filtering dispersion.

(Reproduced with permission from Ref. [19]).

In an alternative approach, Bose *et al.*[^20] achieved the exfoliation of graphite in water, based on the non-covalent interaction between graphene and 9-anthracene carboxylic acid (ACA). The yield of the sample was about 2.3 %. This method (Figure 3) needs no strong acids, oxidants or hydrazine, which could distort the C-sp² network of graphene, and is carried out at room temperature, opening the way to technological applications where the
temperature range is limited. Raman spectroscopy of the functionalized graphene (ACA-G) confirmed the abundant presence of superior quality single layers. The excellent dispersion stability of ACA-G was corroborated by absorption spectroscopy. Cyclic voltammetry measurements of an ACA-G-based ultracapacitor demonstrated excellent capacitive behaviour, with a high specific capacitance value of 148 F g\(^{-1}\).

Recently, Spyrou and co-workers\(^{[21]}\) performed experimental and theoretical studies in order to explain the intercalation mechanism of polycyclic aromatic molecules (aromatic amines) into graphene oxide. The type of interaction differs depending on the size of the aromatic molecule (aniline and naphthalene amine); more specifically, it was shown that aniline binds covalently to the graphite oxide matrix, while naphthalene amine prefers to adsorb on the GO surface via \(\pi-\pi\) interactions. This novel class of hybrid materials opens new horizons in intercalation chemistry and may drive potential applications in electronics, energy storage and environmental remediation.

**Figure 3:** Proposed mechanism for the formation of stable aqueous dispersion of graphene. (Reproduced with permission from Ref. [20]).
A simple and low-cost path for the generation of stable aqueous dispersions of conducting polymers for sensing applications was developed by Liu et al.[22]: interface polymerization of 3,4-ethylene dioxythiophene (EDOT) in the presence of graphene oxide (GO) resulted in PEDOT nanorods-GO nanocomposites. The formation of the composite relies on π-π stacking interactions as well as the electrostatic interactions between the positively charged poly(3,4-ethylene dioxythiophene) (PEDOT) and the negatively charged graphene oxide (GO). Graphene oxide acts as a suitable stabilizing agent for PEDOT due to its abundance in hydrophilic groups. It has been proven that PEDOT displays a high catalytic activity for the oxidation of nitrite. For this reason, Liu et al.[22] successfully designed a nitrite sensor, depositing the stable aqueous dispersion of PEDOT-GO nanocomposites on a Au electrode surface in the presence of Chitosan. Cyclic Voltammetry measurements demonstrated that in such a device the linear detection range and the detection limit amount to 4 μM to 2.48 mM (r=0.999) and 1.2 μM at a signal-to-noise ratio of 3, respectively.

The first attempt to develop polyvinyl alcohol (PVA) composites based on pristine graphene was performed by Das et al.[23] who dispersed pristine few-layer graphene (FLG) in water in the presence of a triphenylene based stabilizer (C10). The surface of FLG was functionalized by C10 without micelle formation and the C-sp² network was not disrupted. A high graphene yield was obtained (0.2 mg FLG/mg C10) and the stability of the product was not affected by pH changes, heat and freeze-drying. The FLG/PVA composites exhibited enhanced mechanical and electrical properties, namely the electrical conductivity of the FLG/PVA composite (0.29 vol%) was much higher than that of a pure PVA film and in the case of 0.1 vol% (0.3 wt%) FLG/PVA composite the Young’s Modulus was increased by 21 %. Such improved behaviour demonstrates excellent percolation between filler and matrix as well as effective reinforcement and promises well for the application of stabilized pristine graphene in conductive composite films.
Sun et al.\cite{24} studied the adsorption of PAHs (naphthalene, anthracene and pyrene) on graphene oxides (GOs) and reduced graphene oxides (rGOs) and tried to evaluate the effect of pH, humic acid (HA) and temperature on the adsorption of PAHs on graphene nanomaterials. They found that the adsorption of PAHs on rGOs was not affected by the increase of pH, from 2 to 11. On the other hand, in the case of naphthalene on rGOs, the adsorption was suppressed by high temperatures and by the presence of humic acid. The saturated adsorption capacities (in mmol g\(^{-1}\)) of rGOs for PAHs, calculated with the Polanyi-Dubinin-Ashtahhov model (PDA) gave the highest value for naphthalene, followed by pyrene and anthracene and the adsorption isotherms of the three samples were in accordance with this model. Concerning the adsorption mechanisms of PAHs on rGOs, the authors found that in the case of naphthalene, the adsorption was realized via pore-filling, whereas for anthracene and pyrene it proceeds through adsorption on the flat surface.

Only a year later, Wang, Chen and Chen\cite{25} studied the influence of the PAH size and hydrophobicity on the interaction with GO and graphene, choosing again naphthalene, anthracene and pyrene as adsorbants. The binding of PAHs to graphene is dominated by \(\pi-\pi\) interactions on the flat surface and the possibility to interact with more than one surface in the groove regions formed by wrinkles on the graphene surface. While the perfect 2D graphene structure tend to alter into 3D structures to become structurally stable, GO forms much fewer wrinkles because the attached carboxyl groups already stabilize the structure. As illustrated by the TEM and SEM images reproduced in Figure 4, the conformation of the starting materials is therefore different but for both graphene and GO the conformation and aggregation of the nanosheets is severely altered after loading with PAHs. The authors make various hypotheses about the underlying mechanisms but further studies are needed to discriminate between these scenarios.
**Figure 4:** The SEM and TEM images of graphene (GNS) and graphene oxide (GO) before (first column) and after association with phenanthrene at a low concentration (second column) and at a high concentration (third column). (Reproduced with permission from Ref. [25]).
Finally, Xin Yang et al.[26] studied the adsorption of 1-naphthylamine, 1-naphthol, and naphthalene on reduced graphene oxide/iron oxide (GO/FeO•Fe₂O₃) nanocomposites with different polarity (Figure 5). The adsorption capacity of these aromatic molecules on FeO•Fe₂O₃ was much lower than on GO/FeO•Fe₂O₃ composites because the van der Waal forces between naphthalene or naphthalene derivatives and FeO•Fe₂O₃ nanoparticles are weaker. Most of the aromatic molecules were adsorbed directly on the surface of GO. The interactions of the magnetic graphene hybrids and aromatic systems were found to be of electron-donor-acceptor (EDA) type and the adsorption capacity increased with increasing dipole moment (naphthalene < 1-naphthol < 1-naphthylamine). Thermodynamic experiments further indicated that the adsorption processes were endothermic and spontaneous. The iron oxide nanoparticles avoid strong aggregation and
facilitate separation for an easy removal. All these results are of great interest for applications where highly toxic and carcinogenic aromatic molecular systems need to be removed from the environment.

### 3.4 Electronic and electrochemical properties of graphene/PAHs hybrids

As already mentioned above, PAHs can be considered as small truncated graphene sheets and PAHs-graphene hybrids are proposed as potential materials for nanoelectronic applications and electrochemical biosensors. An effort in this direction was made by Jo et al.\[^{27}\] who realized the non-covalent functionalization of reduced graphite oxide with poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) and proved the potential of this hybrid for application as transparent and highly flexible electrode. The RGO/PEDOT dispersion maintained good colloidal stability in aqueous media. After filtration the resulting RGO/PEDOT film could be transferred onto a substrate, such as a flexible PET or a quartz slide, and displayed a high conductivity of 2.3 kΩ/sq and an optical transmittance of 80%. The method followed conserves of the chemical and electronic properties of both components while taking advantage of conducting network structure of the conducting polymers to enhance the flexibility and mechanical stability of the reduced graphene oxide sheets.

An electrochemical biosensor where a graphene-nafion hybrid is part of a layered structure, was developed by Yongnian Ni et al.\[^{28}\] for the analysis of benzo(a)pyrene (BaP). This PAH consists of five benzene rings and its metabolites are mutagenic and highly carcinogenic. The sensor consists of DNA immobilized on hemin on top of a nafion-graphene hybrid, deposited on a glassy carbon electrode (GCE). After deposition the nafion-graphene film appeared to have a fibrous structure, which was successively covered by a disordered layer of hemin and DNA. To investigate DNA damage, the
DNA/hemin/nafion-graphene/GCE was immersed separately in solutions of BaP, H₂O₂ and BaP-H₂O₂. Electrochemical impedance spectroscopy technique revealed the damage caused by a metabolite of BaP and UV-Vis spectrophotometry was applied to investigate whether the hemin/H₂O₂ system could mimic the benzo(a)pyrene enzymatic effects. The results showed that this model system could successfully metabolize the BaP PAH molecule to its ultimate carcinogenic form.

Shan Liu et al.[29] constructed an electrochemical sensing platform by modification of electroactive thionine-functionalized graphene onto a glassy carbon electrode surface (Th/GRs/GCE) in order to selectively detect specific polycyclic aromatic tricyclic hydrocarbons, such as phenanthrene (PHE) and anthracene (ANT). To construct the sensing platform, graphene oxide (GO) was synthesized according to Hummers method and the modified electrode prepared from a glassy carbon electrode added in solution of nafion and Th/GRs. UV-Vis absorption spectrum suggested interactions between amino groups of thionine and graphene, as well as π-π stacking. The electrochemical results showed that the modified electrode Th/GRs/GCE retained the electrochemical properties of thionine; it proved stable, reproducible and insensitive with respect to inorganic ions, which are likely to be present in water samples. Analysis of the effect of PHE and ANT on the electrochemical behaviour of Th/GRs/GCE showed that the modified electrode presented a similar response in both cases and that the influence of the coexistence of PHE and ANT was equivalent to the effect of stacking. The modified electrode can be also employed to determine the total amount of PHE and ANT with superb accuracy as proven by successfully measuring the content of PHE and ANT in a standard liquid sample containing 16 PAH compounds. This sensitive electrochemical technique can selectively detect tricyclic aromatic hydrocarbons with carcinogenic and mutagenic properties or occurring as pollutants in the environment.[30]
Bai et al.\[31\] succeeded in stably dispersing single layer graphene sheets in water by non-covalent functionalization with sulfonated polyaniline (SPANI). After reduction of exfoliated graphite oxide by the presence of SPANI, the composite film of SPANI-functionalized graphene sheets (SPANI/r-G) exhibited enhanced electrochemical stability and improved electrochemical activity (Figure 6) in both acidic and neutral media.

![Cyclic voltammograms of SPANI (dashed line) and SPANI/r-G (solid line) modified electrodes in 1.0 M H\textsubscript{2}SO\textsubscript{4} and 0.1 M PBS. Potential scan rate = 50 mV s\textsuperscript{-1}. (Reproduced with permission from Ref. [31]).](image)

### 3.5 Elimination of aromatic organic pollutants using graphene

As already mentioned, polycyclic aromatic compounds are of big concern for the environment\[9\] because many of them are highly toxic, mutagenic and carcinogenic.\[32-35\] Graphene as a non-toxic compound is ideally suited for the absorption and subsequent removal of noxious PAHs from the environment including aquatic systems.

While the exceptionally high surface area of graphene (theoretical estimated value of 2620 m\textsuperscript{2}/g) and its consequently high adsorption capacity make it very promising for the treatment and management of organic and PAHs pollutants, however, the strong tendency towards aggregation of graphene sheets, which reduces the surface area as well as the lack of effective ways to disperse...
graphene in aqueous solution, have been major challenges. In order to overcome these difficulties many approaches have been suggested and the most interesting ones are discussed in detail in this review.

In 2010 Luo et al. developed a new poly(ethylene glycol dimethacrylate)/graphene composite by in-situ polymerization using microwave irradiation. The new composite was used as extraction coating in stir rod sorptive extraction for the preconcentration of polycyclic aromatic hydrocarbons from aqueous samples. The performance of these hybrid composites as sorbents was compared to that of the pure polymer in stir rod sorptive extraction and the graphene-polymer composite proved to have a higher extraction capacity for most target PAHs from aqueous samples.

Aiming to develop a new class of adsorbents with high adsorption capacity for persistent organic pollutants, in 2011 Zhao et al. introduced a type of sulfonated graphene, which was dispersible and capable of absorbing aromatic pollutants from aqueous solutions. Graphene oxide, prepared by a modified Hummers method, was pre-reduced by adding sodium borohydride, sulfonated with aryl diazonium salt of sulfanilic acid and then post-reduced with the help of hydrazine to remove any remaining oxygen functionalities. The adsorption capability of the sulfonated graphene nanomaterials was found to be ~2.3–2.4 mmol g⁻¹ for naphthalene and 1-naphthol, which is among the highest for today's nanomaterials.

Two years later in 2013, Qiang et al. developed a new graphene-based solid phase extraction disk for the separation and pre-concentration of polycyclic aromatic hydrocarbons from aqueous samples. The method was tested using Gas chromatography–mass spectrometry. Solid phase extraction is a commonly used treatment method for environmental samples, so the demonstration that graphene has a strong adsorption capacity for PAHs identifies it as an excellent and cost-effective adsorbent material for separating PAHs from water samples.
In the same year, Zhang et al.\cite{39} developed a novel non-covalently bound hybrid material by mixing graphene oxide and brilliant blue. This new type of functional graphene oxide was efficiently dispersed and stable in water rendering it attractive for the absorption of polycyclic aromatic hydrocarbons such as anthracenemethanol and fluoranthene. In both cases the brilliant blue-GO hybrid exhibited similarly high adsorption capacity as the sulfonated GO cited above. In addition the authors developed a new solid-liquid separation method to remove PAH-charged hybrid material without the addition of any flocculant.\cite{39} By controlling pH and temperature, the PAH-charged complexes were successfully removed through coagulation without the need to introduce any further treatment (filtration or centrifugation).\cite{39}

A different approach was followed by Fang Wang and co-workers\cite{40} who performed a series of adsorption experiments using colloidal graphene oxide nanoparticles. They proved that compared to other carbon nanomaterials like carbon nanotubes and fullerene, GO nanoparticles exhibited a stronger adsorption capacity not only for very hydrophobic organic contaminants but also for hydrophilic, polar organic contaminants (pyrene, phenanthrene, naphthalene, 1,3-dichlorobenzene, 1-naphthol, 1-naphthylamine, 2,4-dichlorophenol, and 2,4-dinitrotoluene). The authors measured contaminant concentrations in the aqueous phase by applying the negligible depletion-solid-phase microextraction (nd-SPME) method and found that GO nanoparticles were a much more effective contaminant carrier than other types of carbon nanomaterials because they were highly stable and better dispersible.\cite{40}

3.6 Graphene/PAHs nanocomposites with enhanced thermal conductivity and mechanical properties

Graphene can also be added as filler in polymer composites to enhance the thermal conductivity and improve the mechanical properties. Teng et al.\cite{41} proposed a new approach for realizing such a composite through the non-
covalent functionalization of pyrene with a functional segmented poly(glycidyl methacrylate) (Py-PGMA) on thermally exfoliated graphene. The Py-PGMA was prepared by atomic transfer radical polymerization, which improves the compatibility between graphene and epoxy matrix due to the reactive pendant oxirane rings. Py-PGMA grafted on graphene (Figure 7) engenders the homogeneous dispersion of the graphene flakes in polymer composites, increasing the contact surface area between the Py-PGMA-functionalized graphene and the polymer.\[^{[41]}\]

![Diagram](image)

**Figure 7:** Schematic representation of preparation and functionalization of graphene for use as a filler in polymer composites. (Reproduced with permission from Ref. \[^{[41]}\].)

An alternative approach has been presented by Tang *et al.*\[^{[42]}\] who developed a novel non-covalent strategy based on cationic dye rhodamine B (RhB) which functionalizes graphene by *in-situ* reduction to obtain dispersed colloid graphene. The dye interacts with graphene by cation-\(\pi\) and \(\pi-\pi\) interaction preventing in such way the aggregation of graphene, and incorporated into polyvinyl alcohol allows to fabricate high performance PVA/graphene composites with enhanced mechanical properties by simple solution casting.\[^{[42]}\]
With the addition of RhB-graphene, the strength and flexibility of the composites were simultaneously improved and a spectacular reinforcing effect was observed.\textsuperscript{[42]}

In 2013, Sung Ho Song and his group\textsuperscript{[43]} introduced a novel graphite intercalation approach to generate graphene flakes (GFs) by using a ternary eutectic system of alkali salts and fabricated high quality GFs with extremely low oxygen content to be utilized in polymer composites for thermal management and thermal conductivity enhancement.\textsuperscript{[43]} The authors suggested a protocol for obtaining non-covalently functionalized GFs with 1-pyrenebutyric acid (PBA) that are highly soluble in various solvents and can be used to synthesize an epoxy-graphene composite. This highly effective and non-destructive method allows to obtain non-oxidized and low-defect GFs, which at low loading levels are more effective fillers than GO and MWNTs for producing polymeric nanocomposites with high thermal conductivity (Figure 8).\textsuperscript{[43]}

\textbf{Figure 8:} Schematic representation of experimental procedure a) graphene flakes produced through intercalation a ternary eutectic system of alkali salts and dispersed in pyridine, b) graphene flakes non covalently functionalized by PBA and dispersed in acetone, c) Curing Agent, and functionalized graphene flakes after sonication, d) fabrication nanocomposites with functionalized graphene flakes by curing for 1 h at 175 °C. (Reproduced with permission from Ref. [43]).
Wen-Shi Ma et al.\textsuperscript{[44]} introduced a novel procedure to prepare non-covalently modified graphene nanosheets by reduction of graphene oxide with hydrazine hydrate and simultaneous non-covalent functionalization via 1-allyl-methylimidazolium chloride (AmimCl) ionic liquid. AmimCl is assumed to interact with graphene by cation–\(\pi\) stacking and \(\pi–\pi\) interaction as well as electrostatic repulsion preventing aggregation between graphene nanosheets.\textsuperscript{[44]} Ionic liquid-modified graphene (IL-G) nanosheets were well-dispersed and individually exfoliated in a mixture of DMF and butyl acetate and then incorporated into polyurethane (PU) to fabricate IL-G/PU nanocomposites by solution blending (Figure 9). Great improvements in both mechanical and thermal properties of the final nanocomposites properties were achieved at a low loading of IL-G nanosheets.

\textbf{Figure 9:} Schematic representation of nanocomposites with ionic liquid-modified graphene as a filler. (Reproduced with permission from Ref. [44]).

On the theory side, Shangchao Lin and Markus J. Buehler\textsuperscript{[45]} introduced a less destructive non-covalent functionalization method which attempts to enhance the thermal performance of graphene/organic nanocomposites and
used molecular dynamics (MD) to simulate it. Towards this end, they designed alkyl-pyrene molecules that can non-covalently functionalize graphene surfaces in contact with a model organic phase composed of octane. A physically adsorbed layer of linkers to the graphene/octane interface results able to bridge the vibrational mismatch at the graphene/octane interface.[45]

3.7 Conclusions

In conclusion, the aim of this mini-review was to present the most innovative theoretical and experimental work concerning the interaction of polycyclic aromatic molecules with graphene sheets. These studies are very crucial considering the role of PAHs in the development of novel composites for electronic, sensing and biomedical devices, but they are also of great importance for environmental remediation, given the high level of toxicity of PAHs when dispersed in the environment. PAHs and their metabolites have been identified as mutagenic and carcinogenic so their elimination with the help of nanomaterials like graphene is mandatory for the safeguard of living organisms.
References


