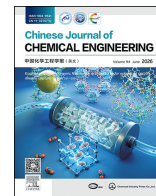




Contents lists available at ScienceDirect

Chinese Journal of Chemical Engineering

journal homepage: www.elsevier.com/locate/CJChE

Full Length Article

Investigating the capabilities of nano-sized graphene and graphene oxide to be a nanosorbent for mixed pesticides in solution: MD simulation study

Prin Tadawattana¹, Sirin Sittiwanchai¹, Kyohei Kawashima², Jitti Niramitranon³, Toshifumi Mori^{2,4,*}, Prapasiri Pongprayoon^{1,5,*}¹ Department of Chemistry, Faculty of Science, Kasetsart University, Chatuchak, Bangkok 10900, Thailand² Institute for Material Chemistry and Engineering, Kyushu University, Kasuga, Fukuoka 816–8580, Japan³ Department of Computer Engineering, Faculty of Engineering, Kasetsart University, Chatuchak, Bangkok 10900, Thailand⁴ Interdisciplinary Graduate School of Engineering Science, Kyushu University, Kasuga, Fukuoka 816–8580, Japan⁵ Center for Advanced Studies in Nanotechnology for Chemical, Food and Agricultural Industries, KU Institute for Advanced Studies, Kasetsart University, Bangkok 10900, Thailand

ARTICLE INFO

Article history:

Received 8 October 2025

Received in revised form

25 January 2026

Accepted 1 February 2026

Available online 7 March 2026

Keywords:

Pesticides

Molecular dynamics simulation

Nanoscale graphene

Oxygen contents

Graphene quantum dot

Pesticide adsorption

ABSTRACT

Pesticide contamination is a growing global environmental concern. Among various remediation methods, adsorption from wastewater remains one of the most cost-effective strategies. Graphene-based nanomaterials have been identified as promising candidates for this purpose. Recently, nano-scale graphene oxide (GO) has attracted interests due to its size compatibility with pesticide molecules, good biocompatibility, and low cytotoxicity, making it a potential pesticide sorbent. While a previous study revealed the adsorption mechanisms of individual pesticides (cyfluthrin (CFT), diazinon (DZ), and ivermectin (IVM)) onto nanoscale GO, the adsorption of mixed pesticides remains underexplored. This study investigates the adsorption of mixed pesticides (CFT, DZ, and IVM) onto GO with varying oxygen contents (25% (GO25) and 40% (GO40)) compared to pristine graphene (PG) using Molecular Dynamics (MD) simulations. The results reveal spontaneous competitive pesticide adsorption on all surfaces driven by alkyl- π and π - π interactions with the graphene-like regions. PG shows the most effective sorbent, while GO40 is the worst resulting in the highly shuffling motion of pesticides. IVM exhibits the strongest affinity across all materials and shows the highest surface occupancy, with its binding behaviour unaffected by oxygen content. In contrast, the CFT and DZ adsorption varies with GO oxygenation levels suggesting that surface functionalization can be tuned to selectively target specific pesticides. Pesticide clustering is also observed. IVM acts as a central anchor molecule through alkyl- π and π - π interactions and hydrogen bonds. These findings highlight the potential of nanoscale graphene materials as customizable sorbents for pest control.

© 2026 The Chemical Industry and Engineering Society of China, and Chemical Industry Press Co., Ltd. All rights are reserved, including those for text and data mining, AI training, and similar technologies.

1. Introduction

Pesticide is a substance or mixture of substances used to prevent, repel, or mitigate any pest including fungi, insects, weeds, and rodents [1–3]. Pesticides are used in various settings such as

agriculture, homes, and public health programs. Some pesticides are incorporated with metals (e.g. lead, copper, cadmium, and zinc) [4,5] or metal oxides for specific actions (inorganic pesticide); however, its contaminants are toxic to living organisms and environment [4]. Organic pesticides were reported to be less toxic, simply degradable than some inorganic substances [6]. Therefore, organic pesticides have been widely used instead of inorganic chemicals. To date, commonly used organic pesticides are divided into four main groups, i.e., organophosphates, organochlorines, pyrethroids, and carbamates [7]. Although small amounts of pesticides are needed for pest control, their contamination from environmental sources remains an issue. Farmers usually employ

This article is part of a special issue entitled: Sino-Thai Frontiers of Green Chemical Engineering published in Chinese Journal of Chemical Engineering.

* Corresponding authors.

E-mail addresses: fsciprpo@ku.ac.th (T. Mori), toshi_mori@cm.kyushu-u.ac.jp (P. Pongprayoon).

<https://doi.org/10.1016/j.cjche.2026.02.002>

1004-9541/© 2026 The Chemical Industry and Engineering Society of China, and Chemical Industry Press Co., Ltd. All rights are reserved, including those for text and data mining, AI training, and similar technologies.

the overdose of pesticides to obtain high agricultural productivity, but they are not aware that using excess pesticides causes more poisonous contamination unfit for consumption. The pesticide contamination can lead to serious health issues, including genetic mutations, cancers, neurotoxicity, endocrine disruption, and reproductive disorders [7–10]. Excess pesticides persist in the environment and pose a hazard to living organisms, especially humans [7]. Due to the significant health risks to humans, numerous efforts have been made to monitor and detect pesticide residues in the environment and agricultural products.

Recent studies have explored the methods for detecting excess pesticide residues [11]. Graphene-based materials, particularly graphene oxide (GO), have demonstrated strong potential for pesticide removal from wastewater due to their large adsorption surface area and thermal and pressure stability [12–15]. GO can be functionalised to target specific contaminants, and its natural abundance suggests a potential for cost-effective application [16]. GO also has high specific surface area, providing abundant adsorption sites [17]. Thus, GO has become a promising tool in environmental remediation technologies. Traditional spectroscopic techniques such as liquid chromatography-mass spectrometry (LC-MS) and gas chromatography-mass spectrometry (GC-MS) are commonly used for pesticide quantification. Nonetheless, these methods need sophisticated instruments and trained personnel, making them impractical for on-site or field applications. Consequently, many studies have focused on developing rapid, sensitive, and portable sensor technologies where GO has played a significant role in the design and development [18–20]. Furthermore, GO has been used as a sorbent due to its high efficiency in pesticide adsorption and its recyclability [21–23]. The mechanism of pesticide aggregation on GO has been extensively investigated [22,24], with π - π stacking interactions identified as the primary driving force behind the adsorption process [14,22,24]. Notably, most prior studies have used micro-sized GO and graphene materials as pesticide sorbents. Recently, nano-sized GO or graphene quantum dot (GQD) with sizes below 100 nm has attracted attention due to its high biocompatibility and low cytotoxicity [25,26]. Nanoscale GOs or GQDs are particularly promising for sensing applications because of their unique optical and electronic properties [25,27,28]. In addition, GQDs have been experimentally employed for pesticide detection and small-molecule sensing [29–32]. It was found that while micro-sized GO exhibited toxicity and even caused mortality in mice, nano-sized GO or GQD had no apparent harmful effects [25]. Another study reported that nano-sized GO had minimal impact on human hematopoietic stem cells after 36 h incubation. Importantly, the nanoscale dimension of GO, which is comparable to the size of pesticides, makes it particularly attractive for enhancing adsorption performance and for future applications in pesticide removal or delivery systems.

Recently, nano-sized GO with 25% oxygen contents has shown the capability to collect organic pesticides (cyfluthrin (CFT), ivermectin (IVM), diazinon (DZ)) from different families (pyrethroid, avermectin, and organophosphate families) [33]. These are the major pesticides that have a serious impact on humans and animals [34–38]. All pesticides were found to spontaneously adhere on GO at a graphene-like region *via* the π - π and π -alkyl interactions, where each pesticide exhibited different binding affinities [33]. IVM acts as the best adsorbate for nano-sized GO *via* both dispersion and hydrogen bonds [33]. Yet, no effect of mixed pesticides on GO binding was investigated. In practice, a mixture of pesticides is found in the environment, so the binding of mixed pesticides to nano-sized GO is an interesting topic to explore the feasibility of using the nanoscale GO to remove or collect pesticides from the environment. Also, the effect of oxygen content ratio on the pesticide-GO clustering remains unclear.

Therefore, in this study, the effects of mixed pesticides and the oxygen contents (%) of nano-sized GO on pesticide-GO aggregation are investigated. Molecular Dynamics (MD) simulations were conducted to study the aggregation of pesticides and nano-sized GO. A nanoscale GO model was constructed based on the Lerf-Klinowski model, using the most stable configuration with 2:1 ratio of hydroxyl ($-\text{OH}$) to epoxy ($-\text{O}-$) groups [39]. Nanoscale GO models with 25% and 40% oxygen contents were employed (Fig. 1A). The 25% oxygenation ratio was used here because it provides an optimal balance of functional group and structural stability for adsorption [40,41], while the 40% oxygen content represents a highly oxidised, but still structurally stable [42,43]. A nanoscale pristine graphene (PG) was also studied as a reference. A mixture of six commonly used pesticides (two each of cyfluthrin (CFT), ivermectin (IVM), diazinon (DZ)) was selected to represent three main classes of organic pesticides (Fig. 1B and Fig. S2D in Supplementary Material). Six pesticides included in each system are adequate to surround the GO sheet in all dimensions (Fig. 1C), thereby mimicking the random orientations of the pesticides in solution. Given that GO has previously been employed as a pesticide carrier [14,44], the adsorption insights obtained from this work may contribute to the development of new strategies for both pesticide removal and delivery.

2. Materials and Methods

2.1. Preparation of nano-sized graphene and pesticides topologies

Three types of nano-sized GO models (pristine graphene (PG), and graphene oxide with 25% (GO25) and 40% (GO40) oxygen content) were constructed using HierGO [45]. Each contains 72 carbon atoms with a dimension of 1.5 nm $\times$ 1.3 nm. For GO25 and GO40, a ratio of hydroxyl ($-\text{OH}$) and epoxy ($-\text{O}-$) groups was 2:1 based on the Lerf-Klinowski model [39]. All graphene models were optimised using Density Functional Theory (DFT) at the B3LYP-6-31G(d) level using Gaussian 16 software package [46]. The restrained electrostatic potential (RESP) charges were obtained by Hartree-Fock calculation at a HF-6-31G(d) level. All topologies were transformed to gromacs format using Antechamber module in AmberTools20 [47]. The three-dimensional structures of cyfluthrin (CFT), diazinon (DZ), and ivermectin (IVM) were generated using Discovery Studio 2021 [48] and parameterized with ACPYPE [49]. All pesticide topologies were built using the AMBER14SB force field. For each system, one nano-sized graphene material (PG, GO25, and GO40) was placed at the centre of a simulation box with a dimension of 6 nm $\times$ 6 nm $\times$ 6 nm. The graphene model consists of a single graphene nanosheet immersed in aqueous solution. This setup is intended to capture the fundamental intermolecular interactions between pesticide molecules and a carbon surface, rather than to represent a full dispersion of nano-sized graphene sheets. Two molecules of each pesticide (cyfluthrin (CFT), diazinon (DZ), and ivermectin (IVM)) were then placed at least 1 nm away from both the graphene sheet and each other to ensure unbiased initial configurations (Fig. 1C). Each system was soaked in the TIP3P water molecules. In total, 3 systems were built, *i.e.*, pristine graphene with six pesticides, GO25 with six pesticides, and GO40 with six pesticides, hereafter denoted as PG-6P, GO25-6P, and GO40-6P, respectively.

2.2. Simulation protocols

All Molecular Dynamics (MD) simulations were calculated using GROMACS2022.7 software package [50]. The Particle mesh Ewald (PME) [51] at 1 nm radius cutoff, 0.12 nm Fourier spacing,

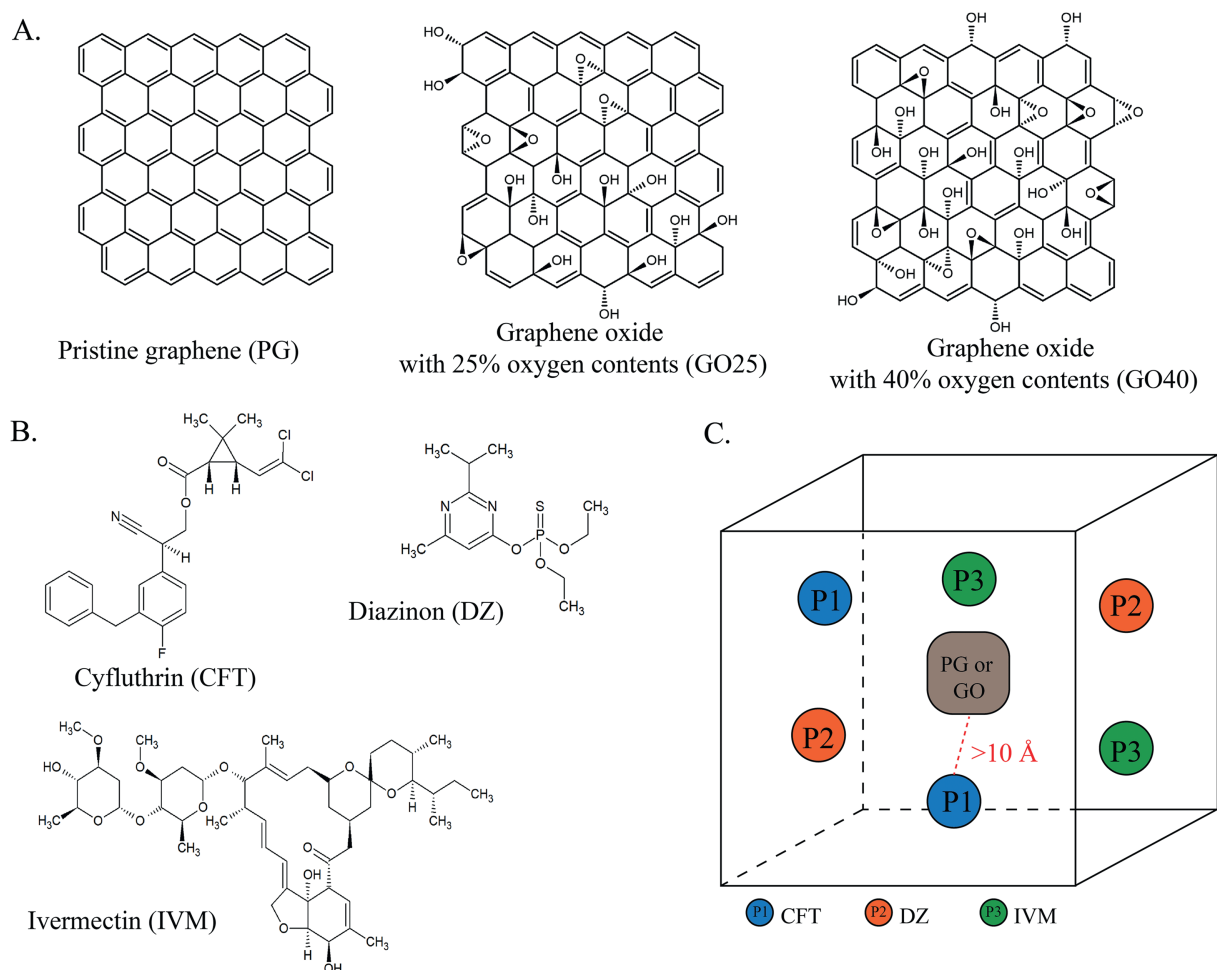


Fig. 1. (A) Chemical structures of nanoscale pristine graphene (PG), graphene oxide with 25% oxygen contents (GO25), and 40% oxygen contents (GO40). (B) Structures of cyfluthrin (CFT), diazinon (DZ), ivermectin (IVM). (C) Locations of pesticides in all systems. Pesticides were randomly placed at least 1 nm away from GO. Each bead (P1–P3) represents each pesticide (P1, P2, and P3 are CFT, DZ, and IVM, respectively).

and fourth-order spline interpolation was used for electrostatics treatment. The bond lengths within each system were constrained by LINCS method [52]. All systems were set in the periodic boundary in all directions. Simulations were carried out under isothermal-isobaric (NPT) conditions, maintaining a constant number of particles, pressure, and temperature. Temperature was regulated at 300 K using the Berendsen thermostat [53] with a coupling time constant of $\tau_t = 0.1$ ps. Pressure was regulated at 1 bar via the Parrinello-Rahman algorithm with a coupling constant of $\tau_p = 1$ ps. The integration time step was set to 2 fs, and trajectory coordinates were recorded every 2 ps. Prior to the production run, energy minimization was carried out using the steepest descent algorithm for 1000 steps to eliminate bad contacts. This was followed by a 10–ns equilibration and a 1– μ s production run. System equilibration was verified by monitoring the time evolution of temperature, pressure, and total energy. Equilibrium was confirmed when these properties fluctuated stably around their target values without systematic drift (Fig. S1 in Supplementary Material).

All presented graphical images in this work were built by Discovery Studio 2021 [48] and Visual Molecular Dynamics (VMD) [54]. The number of hydrogen bonds were counted based on the hydrogen-donor-acceptor cutoff angle at 30° and radius at

0.35 nm. The Poisson-Boltzmann solver (MM-PBSA) option in GROMACS as “*gmx_mmpbsa*” [55] was used to calculate the binding energies of graphene-pesticides and between pesticides. The percentages of pesticide occupancies were calculated as the number of contacts formed by that pesticide divided by the total number of contacts in the system, multiplied by 100.

3. Results and Discussion

Initially, the aggregation between nanoscale graphene materials and pesticides was observed to occur spontaneously in all cases (Fig. 2A). The presence of oxygen atoms does not hinder with nanoscale graphene-pesticide clustering, but they influence the binding affinities. Pesticides in PG appear to distribute more uniformly across the surface, whereas, in both GO25 and GO40, they preferentially align along the graphene-like areas (Fig. 2B, and Fig. S2 in Supplementary Material). These observations are consistent with a previous work reporting that pesticides preferentially adsorb onto graphene-like regions [33]. Moreover, the limited area within these regions promotes pesticide stacking (Fig. 2A). In addition to binding with graphene materials, the self-assembly of individual pesticides on the graphene surface is also observed (Fig. S3 in Supplementary Material). Among the

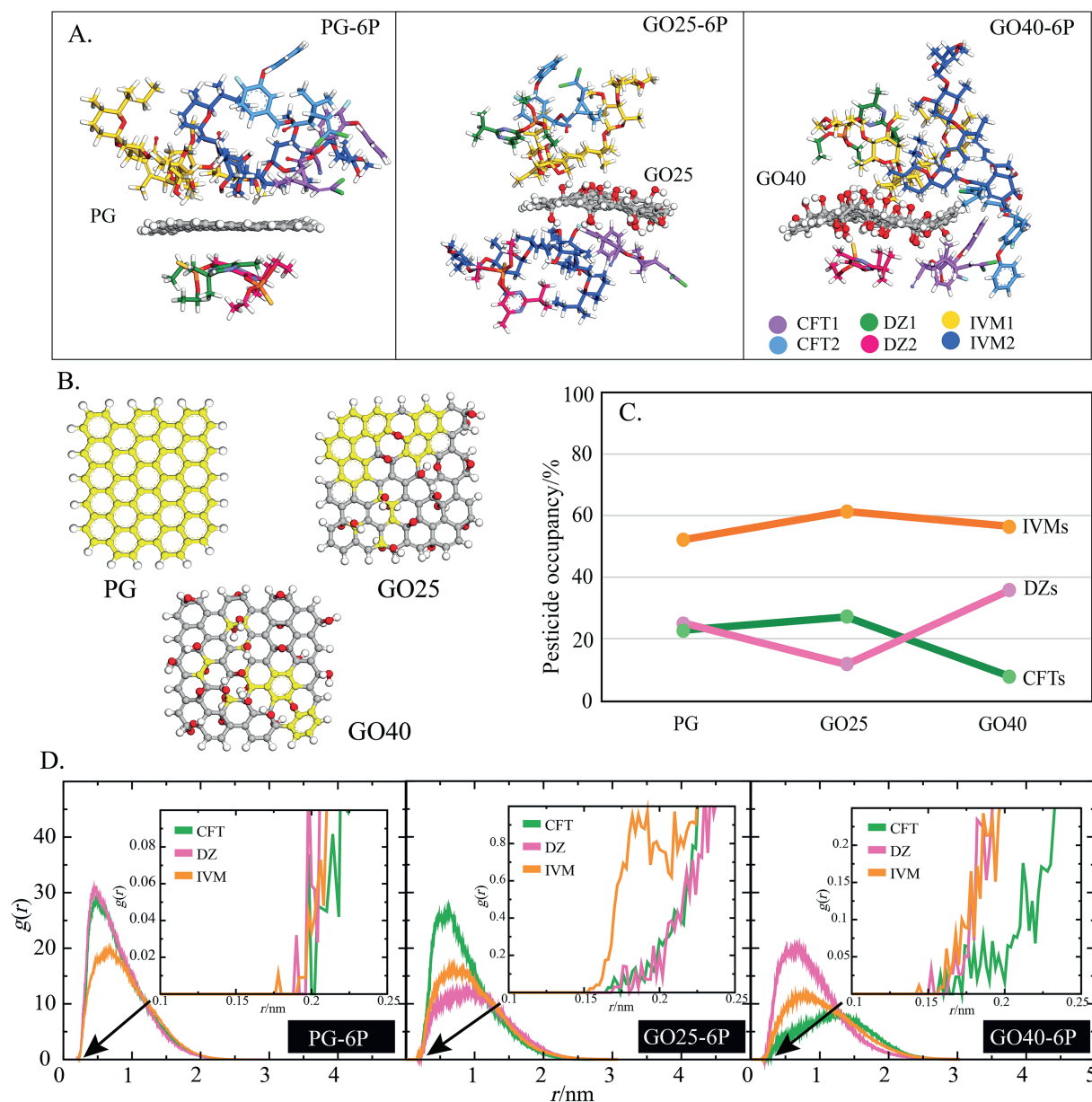


Fig. 2. (A) Final snapshots of all systems (PG-6P, GO25-6P, and GO40-6P). (B) Graphene-like areas in all systems are shown in yellow. (C) Percentages of pesticide occupancies on graphene-based materials (PG, GO25, and GO40). (D) Radial Distribution Function (RDF) of all pesticides.

pesticides studied here, IVM (the largest molecule) exhibits the highest surface occupancy (~50% to 60%) across all systems (Fig. 2C), which is attributed to its ability to form persistent interactions with a graphene surface. In contrast, the smaller molecules, CFT and DZ, display ~25% occupancy on PG but respond differently to GO25 and GO40. GO40 enhances DZ adsorption, suggesting that increased oxygen content improves DZ binding affinity. However, the same oxygen content significantly reduces the CFT adsorption (Fig. 2C). Interestingly, GO25 appears to inhibit DZ binding. IVM appears to be insensitive to the oxygen content, whereas DZ and CFT exhibit oxygen-dependent adsorption behaviours. DZ shows a preference for high oxygen-ratio graphene, while increased oxygenation reduces CFT adsorption (Fig. 2C). Among all pesticides, the radial distribution functions (RDFs) show that IVM has the largest surface occupancy, due to its strong ability

to bind to the graphene surface across all graphene types, particularly in GO25 (Fig. 2D). Interestingly, DZ in GO40 also displays an increased occupancy due to its penetration capability (Fig. 2D). These different degrees of pesticide occupancies and penetrations suggest the competitive adsorption of pesticides. Unlike micro-scale graphene, no “laying-flat” pesticide conformation was observed, likely due to the limited surface area of the nano-sized graphene sorbent. This characteristic may be advantageous for facilitating future desorption. Furthermore, the constantly small radius of gyration (R_g) of PG-pesticide system indicates stable clustering (Fig. S3B in Supplementary Material). In contrast, although pesticides seem to be clustered on the surfaces in GO25 and GO40, the highly fluctuating R_g with occasional large values suggest the dynamic shuffling behaviour in both cases, with pesticides intermittently entering and leaving the cluster during

formation (Fig. S3B in Supplementary Material). Increased oxygenation in GO25 and GO40 likely leads to frequent shuffling of pesticides. Thus, PG appears to be the most effective pesticide sorbent within the three systems studied here.

To explore how each pesticide interacts with the graphene materials, the pairwise contacts between components are analysed (Table 1). The results highlight the competitive adsorption behaviour of all pesticides, with IVM emerging as the most effective adsorbate. This is supported by the high graphene-IVM contacts in all cases (Table 1). For CFT and DZ in PG, their contact numbers are comparable (Table 1). However, the presence of oxygen contents alters the binding affinities of such small pesticides. CFT forms ~28 contacts with GO25, but this number decreases to ~5 contacts with GO40, which contains more oxygens (Table 1). On the contrary, DZ exhibits a preference for GO40 by increasing its contact number from ~12 contacts with GO25 to ~26 contacts with GO40 (Table 1). These observations show that the binding affinities of small pesticides (CFT and DZ) are influenced by the oxygen contents in graphene materials, while IVM remain unaffected due to its ability to interact with both graphene-like and oxygenated regions (Table S1 in Supplementary Material). Thus, varying oxygen levels primarily impact the adsorption of small pesticides like CFT and DZ. These findings also indicate the potential of the nanoscale graphene oxide as a controlled-release adsorbent for

small pesticide molecules. Nonetheless, only about one pesticide-graphene hydrogen bond is formed in GO25 and GO40 (Table 1), as all pesticides tend to favour graphene-like regions (Table S1 in Supplementary Material). The limited number of graphene-pesticide hydrogen bonds observed suggests that pesticide adsorption is driven by hydrophobic interactions. In this context, the binding affinities are influenced by the limited graphene-like surface areas and steric effects common to all pesticides. Due to the limited availability of graphene-like regions, all pesticides tend to aggregate once these regions are fully occupied (Fig. 2A and Fig. S3A in Supplementary Material). The high number of contacts with CFT and DZ suggest IVM, which is the largest molecule, acts as a core to anchor other pesticides onto the graphene surface. Each IVM can interact and form hydrogen bond with other pesticides (Table 1, and Tables S3 and S4 in Supplementary Material). For CFT and DZ, neither self-nor CFT–DZ hydrogen bonds is observed (Table 1). This indicates the aggregation of these pesticides are driven by hydrophobic interactions. However, the more contacts and hydrogen bonds with IVM suggest the binding to IVM is more preferable for CFT and DZ than self- and CFT–DZ aggregation (Table 1 and Fig. S3A and Tables S3–S4 in Supplementary Material). As expected, increased oxygen content in graphene enhances its wettability (Table 1). GO40 exhibits the highest water exposure, whereas the hydrophobic PG shows the lowest. For pesticides, binding to graphene does not significantly affect their water exposure. All pesticides display similar levels of water exposure across all conditions (Table 1). This suggests that the pesticide adsorption is not primarily driven by the degrees of water exposure. The large standard deviations observed in Table 1 is from the dynamic nature of the pesticide-GQD system due to the in-and-out binding events of the pesticides to the nanoscale graphene surface. The block-averaged data (Table S2 in Supplementary Material) can confirm that despite these fluctuations, the system is well sampled, and the reported averages are representative of the true binding behaviour.

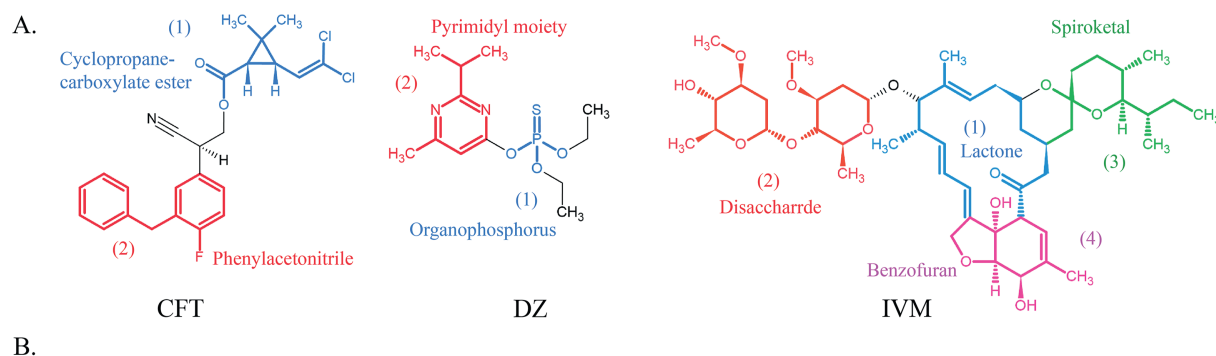
To investigate how each pesticide aligns on a graphene surface, the number of contacts associated with specific pesticide regions are computed (Fig. 3). The results indicate that aromatic groups play a role in graphene-pesticide interactions, while hydrogen bond is minimal (Fig. 3). This implies that the hydrophobic interactions are the main driving force for pesticide adsorption. In PG, CFT interacts with the graphene surface through both cyclopropane-carboxylate ester and phenylacetonitrile moiety (Fig. 3A). However, in GO25 and GO40, the phenylacetonitrile moiety becomes the dominant interacting group (Fig. 3). Similarly, for DZ, the heterocyclic pyrimidyl group is responsible for graphene binding across all graphene types, showing approximately 6–12 contacts (Fig. 3B). Both CFT and DZ show no significant hydrogen bonds with GO25 and GO40 (Fig. 3B). IVM, capable of forming both dispersive interactions and hydrogen bonds, engages all of its structural regions in graphene binding. Nonetheless, consistent with a previous work [33], the non-lactone regions (regions 2 (disaccharide), 3 (spiroketal), and 4 (benzofuran) in Fig. 3A) are the main contributors to IVM adsorption. Notably, in GO25, the benzofuran group of IVM can form a hydrogen bond with the graphene surface (Fig. 3). Overall, in the mixed pesticide system, each pesticide behaves similarly to the case in single-component systems observed in the previous study [33].

Next, the effect of chemical properties of each pesticide on the adsorption capability is investigated *via* the interaction energies between each component (GO-pesticide and pesticide-pesticide) computed by MMPBSA [56] (Table 2). Like the previous studies [24,57–59], the adsorption of all pesticides is driven by vdW interactions. The large size of IVM contributes to its more favourable vdW interaction energies (ranging from –48 to –84 kJ·mol^{–1})

Table 1

Number of contacts (within 0.35 nm) and hydrogen bonds between each component (CFT, DZ, IVM, PG, GO25, GO40, and water) in all systems with standard deviations.

System	Pair	No. of contacts	No. of hydrogen bond
PG–6P	PG–CFT	21.81 ± 17.07	
	PG–DZ	24.04 ± 18.23	
	PG–IVM	49.96 ± 19.78	
	CFT–CFT	11.23 ± 16.16	
	CFT–DZ	4.00 ± 9.49	
	CFT–IVM	19.82 ± 23.72	1.00 ± 0.17
	DZ–DZ	6.88 ± 13.10	
	DZ–IVM	16.87 ± 24.70	1.12 ± 0.22
	IVM–IVM	93.99 ± 32.47	1.03 ± 0.48
	PG–water	176.78 ± 38.34	
	CFT–water	108.88 ± 34.28	1.87 ± 0.96
	DZ–water	146.10 ± 37.21	2.09 ± 1.06
	IVM–water	362.90 ± 71.26	8.57 ± 2.09
GO25–6P	GO25–CFT	28.20 ± 9.79	0.50 ± 0.20
	GO25–DZ	12.12 ± 13.33	0.04 ± 0.21
	GO25–IVM	63.96 ± 16.25	1.32 ± 0.79
	CFT–CFT	2.32 ± 8.24	
	CFT–DZ	6.35 ± 10.89	
	CFT–IVM	31.78 ± 17.36	1.00 ± 0.14
	DZ–DZ	4.43 ± 9.97	
	DZ–IVM	25.52 ± 30.24	1.05 ± 0.27
	IVM–IVM	5.46 ± 12.98	1.02 ± 0.21
	GO25–water	434.90 ± 43.86	21.62 ± 2.67
	CFT–water	95.17 ± 24.59	1.67 ± 0.85
	DZ–water	138.99 ± 36.20	2.00 ± 1.11
	IVM–water	411.41 ± 65.96	9.04 ± 2.04
GO40–6P	GO40–CFT	5.61 ± 10.04	0.52 ± 0.13
	GO40–DZ	25.91 ± 20.46	0.10 ± 0.32
	GO40–IVM	41.00 ± 27.57	0.31 ± 0.47
	CFT–CFT	12.01 ± 13.20	
	CFT–DZ	6.19 ± 11.04	
	CFT–IVM	34.74 ± 23.19	1.00 ± 0.18
	DZ–DZ	12.52 ± 17.59	
	DZ–IVM	22.55 ± 22.20	1.05 ± 0.16
	IVM–IVM	55.40 ± 32.14	1.09 ± 0.34
	GO40–water	528.92 ± 51.47	24.43 ± 3.20
	CFT–water	98.61 ± 32.73	1.66 ± 0.92
	DZ–water	128.57 ± 42.09	1.92 ± 1.05
	IVM–water	380.79 ± 67.13	9.27 ± 2.12



System	Pair	No. of contacts				No. of hydrogen bonds			
		(1)	(2)	(3)	(4)	(1)	(2)	(3)	(4)
PG-6P	PG-CFT	8.51 ± 8.43	9.67 ± 9.48						
	PG-DZ	2.14 ± 2.94	11.47 ± 10.71						
	PG-IVM	19.15 ± 9.65	9.90 ± 10.52	1.55 ± 3.55	18.39 ± 11.38				
GO25-6P	GO25-CFT	7.55 ± 5.61	16.01 ± 7.49			0.05 ± 0.00			
	GO25-DZ	1.16 ± 2.55	6.24 ± 8.06			0.03 ± 0.26	0.01 ± 0.00		
	GO25-IVM	18.31 ± 8.16	4.84 ± 9.21	3.54 ± 5.19	30.30 ± 13.43		0.02 ± 0.18		1.31 ± 0.51
GO40-6P	GO40-CFT	1.88 ± 5.10	6.19 ± 7.40						
	GO40-DZ	3.44 ± 4.92	12.17 ± 10.80			0.07 ± 0.10	0.02 ± 0.00		
	GO40-IVM	8.13 ± 10.86	14.92 ± 16.87	14.92 ± 14.26	2.62 ± 6.51		0.25 ± 0.10		0.04 ± 0.14

Fig. 3. (A) Chemical structures of all pesticides (CFT, DZ, and IVM) where key functional groups are coloured in blue (1), red (2), green (3), and brown (4). In CFT, blue is cyclopropane-carboxylate ester and red is phenylacetone nitrile moiety. In DZ, blue and red are organophosphorus and pyrimidyl moiety. In IVM, blue, red, green, and magenta are lactone, disaccharide, spiroketal, and benzofuran, respectively. (B) Number of contacts and hydrogen bonds between specific regions of pesticide and graphene.

(Table 2). Moreover, the electrostatic energies further support IVM's capacity to bind effectively to both graphene-like and oxygenated regions, particularly in GO25 ($\sim 23 \text{ kJ}\cdot\text{mol}^{-1}$) (Table 2). Nonetheless, similarly to the other pesticides, increasing

Table 2

Average interaction energies ($\text{kJ}\cdot\text{mol}^{-1}$) between each component (PG, GO25, GO40, and Pesticide) with standard deviations in all systems computed by MMPBSA [56]. "vdW" and "Elec" are noted as the van der Waals and electrostatic energies. "Total" is the sum of vdW and Elec values.

System		vdW	Elec	Total
PG-6P	PG-CFT	-50.37 ± 39.99	-3.86 ± 5.28	-54.58 ± 42.96
	PG-DZ	-43.29 ± 35.32	-2.41 ± 6.26	-45.69 ± 35.08
	PG-IVM	-75.88 ± 26.49	-8.45 ± 6.41	-84.34 ± 28.89
	CFT-CFT	-16.20 ± 20.76	-1.97 ± 4.07	-18.18 ± 23.21
	CFT-DZ	-5.11 ± 10.38	-0.73 ± 2.95	-5.84 ± 12.26
	CFT-IVM	-24.23 ± 24.91	-4.50 ± 8.10	-28.73 ± 30.64
	DZ-DZ	-6.98 ± 12.65	-1.42 ± 4.24	-8.39 ± 16.11
	DZ-IVM	-23.97 ± 26.86	-2.97 ± 7.08	-26.93 ± 31.55
	IVM-IVM	-84.28 ± 25.45	-6.99 ± 12.45	-91.27 ± 25.51
GO25-6P	GO25-CFT	-43.93 ± 29.12	-6.36 ± 6.52	-50.29 ± 33.49
	GO25-DZ	-12.00 ± 18.15	-2.57 ± 7.76	-14.57 ± 23.97
	GO25-IVM	-51.53 ± 40.04	-23.57 ± 23.50	-75.11 ± 59.86
	CFT-CFT	-2.92 ± 8.79	-0.49 ± 2.37	-3.41 ± 10.46
	CFT-DZ	-6.03 ± 10.89	-1.01 ± 2.87	-7.04 ± 12.92
	CFT-IVM	-27.82 ± 21.52	-2.47 ± 4.42	-30.29 ± 23.96
	DZ-DZ	-4.42 ± 10.26	-1.05 ± 3.66	-5.47 ± 13.14
	DZ-IVM	-20.03 ± 26.68	-4.03 ± 9.30	-24.06 ± 33.62
	IVM-IVM	-5.64 ± 9.53	-0.05 ± 2.73	-5.69 ± 10.48
GO40-6P	GO40-CFT	-8.02 ± 14.32	-1.33 ± 5.05	-9.35 ± 18.08
	GO40-DZ	-31.30 ± 29.65	-8.24 ± 11.15	-39.54 ± 37.36
	GO40-IVM	-39.78 ± 36.53	-8.30 ± 11.30	-48.07 ± 44.95
	CFT-CFT	-14.84 ± 16.71	-1.54 ± 3.56	-16.38 ± 18.86
	CFT-DZ	-6.16 ± 11.65	-1.15 ± 3.57	-7.31 ± 14.37
	CFT-IVM	-33.55 ± 26.42	-5.25 ± 7.61	-38.80 ± 31.42
	DZ-DZ	-11.68 ± 17.74	-1.43 ± 4.89	-13.11 ± 20.37
	DZ-IVM	-17.73 ± 20.90	-2.34 ± 5.92	-20.05 ± 24.55
	IVM-IVM	-40.36 ± 31.11	-3.45 ± 6.76	-43.81 ± 32.54

the oxygen contents on the graphene surface reduces the vdW interaction energies between graphene and pesticide, resulting in a decrease in their binding affinities. In addition, the high total energies between IVM and the other pesticides in Table 2 supports the idea that IVM acts as a core and anchor other pesticides onto the graphene surface. Compared with the single pesticide-GO25 system in the previous work [33], the comparable size of interaction energies between single-IVM and mixed pesticide systems shows that the competitive adsorption in a mixed pesticide system here does not interfere the binding affinities of IVM (Interaction energies of single-IVM system and mixed pesticides are ~ -77 [33] and $-75 \text{ kJ}\cdot\text{mol}^{-1}$). On the other hand, the solution with mixed pesticide reduces the binding affinities of DZ (interaction energies of single-DZ system and mixed pesticides are ~ -58 [33] and $-14 \text{ kJ}\cdot\text{mol}^{-1}$, respectively), but increases the binding capability of CFT (interaction energies of single-CFT system and mixed pesticides are ~ -40 [33] and $-50 \text{ kJ}\cdot\text{mol}^{-1}$) (Table 2). These findings suggest that the binding affinities of CFT and DZ are influenced by the degree of graphene oxygenation.

Previous studies have shown that, in addition to $\pi-\pi$ interactions, other hydrophobic forces such as alkyl- π interactions contribute to the adhesion on graphene oxide surface [24,57,60–62]. Although π interactions cannot be directly captured by molecular mechanics, they can be inferred from specific structural features such as the planar orientation of aromatic moieties toward the graphene surface (planar angle $\leq 20^\circ$), indicative of $\pi-\pi$ stacking, and a consistent proximity between alkyl chains and the graphene surface, characteristic of alkyl- π interactions [62,63]. Also, recent computational studies suggest that alkyl- π interactions can occur within a carbon-carbon distance of $\sim 0.45 \text{ nm}$ [60,62]. In this work, both $\pi-\pi$ and alkyl- π interactions play vital roles in pesticide adsorption. The structural criteria defining $\pi-\pi$ and alkyl- π interactions, as reported in previous studies, are employed in this work to identify and

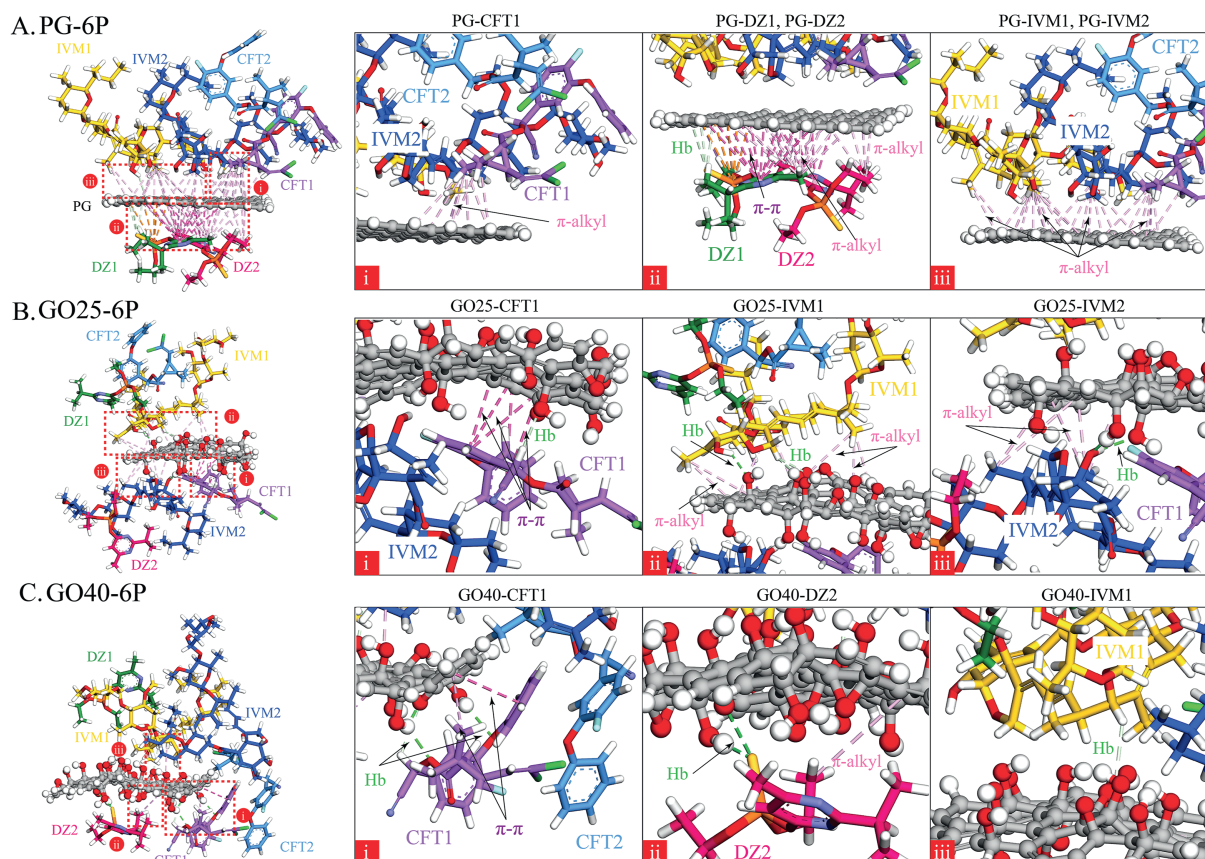


Fig. 4. Orientations of pesticide-graphene complexes in PG-6P (A), GO25-6P (B), and GO40-6P (C). Key interactions between each component are shown as insets (i–iii).

characterize these interactions. Herein, the $\pi-\pi$ stacking and alkyl- π interactions remain the key player for pesticide adsorption. A number of $\pi-\pi$ and alkyl- π interactions are captured (Fig. 4 and Fig. S4 in Supplementary Material). As the level of oxygenation increases, the occurrence of $\pi-\pi$ and alkyl- π interactions decreases due to the disruption of hydrophobic domains. All pesticides in PG seem to show clear aromatic interactions, whereas those in GO25 and GO40 display unstable $\pi-\pi$ and alkyl- π interactions (Fig. S4 in Supplementary Material). It is due to the limited deoxygenated areas in both systems. Such unstable aromatic interactions thus lead to the shuffling motion found here. Each pesticide can also bind to other graphene-bound pesticides through hydrogen bonds, $\pi-\pi$ stacking, and alkyl- π interactions (Table 1 and Fig. S4 in Supplementary Material). Similar to the single-pesticide system [33], IVM remains upright to maintain the hydrogen bonds with the oxygen-rich surface, while smaller CFT and DZ tend to align their core structures along the graphene surface (Fig. 4 and Fig. S6 in Supplementary Material). Even though CFT and DZ can form hydrogen bond and aromatic interactions with oxygenated graphene materials (GO25 and GO40) and IVM (Table 1 and Figs. S4–S5 in Supplementary Material), these interactions are not stable enough to effectively localize pesticides onto the graphene surface. This results in the transient adsorption and desorption of CFT and DZ. In contrast, IVM can bind stably to all graphene types throughout the courses of simulations. Seemingly, the varying degrees of graphene oxygenation appear to influence the adsorption efficiency of smaller pesticides like CFT and DZ. In other words, this highlights the possibility of tuning nano-sized graphene oxide to selectively capture specific pesticide.

4. Conclusions

All nanoscale graphene sheets (PG, GO25, and GO40) enable the rapid and spontaneous adsorption of mixed pesticides (CFT, DZ, and IVM). The average number of pesticide-graphene contacts ranges from 12 to 60 contacts, reflecting preferential interactions with graphitic regions, consistent with previous studies [33]. The $\pi-\pi$ and π -alkyl interactions are the main contributor for pesticide adsorption. Among the materials, PG exhibits the highest adsorption capacity (PG-pesticide contacts of ~22–50 contacts), whereas GO40 performs the worst due to its minimal graphitic character (~6–41 contacts). Competitive adsorption is observed, with IVM showing the fastest and strongest binding (~40–60 contacts) and acting as an anchor for other pesticides, while CFT and DZ affinities are more sensitive to graphene oxygenation levels. These findings demonstrate the strong sorption capability of nano-sized graphene and the tunability of adsorption for smaller pesticides through controlled oxygenation, suggesting potential for sequential extraction. Moreover, compared with micro-sized GO, previously used as a pesticide carrier but associated with toxicity to crops and livestock [14,15], nanoscale graphene materials provide similar adsorption performance with reduced cytotoxicity [64,65]. This highlights the potential as safer alternatives for pesticide management applications. It should be noted that the present model does not account for the concentration of nanoscale graphene or inter-particle competition effects. Therefore, the results primarily provide mechanistic insights into pesticide-graphene surface interactions rather than quantitative adsorption capacities under realistic nanoscale graphene loadings.

CRediT Authorship Contribution Statement

Prin Tadawattana: Writing – review & editing, Writing – original draft, Visualization, Validation, Investigation, Formal analysis, Data curation. Sirin Sittivanichai: Writing – original draft, Methodology, Investigation. Kyohei Kawashima: Methodology. Jitti Niramitranon: Writing – review & editing, Resources. Toshifumi Mori: Writing – review & editing, Writing – original draft, Supervision, Funding acquisition. Prapasiri Pongprayoon: Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Software, Resources, Project administration, Investigation, Funding acquisition, Data curation, Conceptualization.

Declaration of Competing Interest

This manuscript is original, has not been published before and is not currently being considered for publication elsewhere. There are no known conflicts of interest associated with this publication and there has been no significant financial support for this work that could have influenced its outcome.

Acknowledgements

We would like to thank Kasetsart University Research and Development Institute (FF(KU)62.69), Grant-in-Aid for Scientific Research (22H02035, 23K23303, 23KK0254, 24K21756, and 25H02464) from JSPS. The calculations were carried out at Kasetsart University HPC service center (Nontri AI) and the Research Center for Computational Sciences in Okazaki (24–IMS–C105 and 25–IMS–C105).

Supplementary Material

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.cjche.2026.02.002>.

References

- [1] S. Meshram, S. Bisht, R. Gogoi, Current development, application and constraints of biopesticides in plant disease management, *Biopesticides*. Elsevier, 2022.
- [2] M.R. Sultan, S.A. Al Sayed, A.A. Al Farga, Pesticides: classifications, toxicities, and impacts on environment and human health, *J. Food Protect.* 84 (10) (2021) 1422–1434.
- [3] M. Tudi, H. Daniel Ruan, L. Wang, J. Lyu, R. Sadler, D. Connell, C. Chu, D.T. Phung, Agriculture development, pesticide application and its impact on the environment, *Int. J. Environ. Res. Publ. Health* 18 (3) (2021) 1112.
- [4] A.S. Hassan, Inorganic-based pesticides: a review article, *Egypt, Sci. J. Pestic.* 5 (2019) 39–52.
- [5] A. Alengebawy, S.T. Abdelkhalek, S.R. Qureshi, M.Q. Wang, Heavy metals and pesticides toxicity in agricultural soil and plants: ecological risks and human health implications, *Toxics* 9 (3) (2021) 42.
- [6] A. Tudi, S.S. Sharmila, S.K. Maiti, S. Shankar, A. Sharma, R.B. Srivastava, P.K. Singh, Pesticides: types, toxicity, and recent advances in mitigation strategies, *Environ. Chem. Lett.* 19 (1) (2021) 1–25.
- [7] T. Thorat, B.K. Patle, M. Wakchaure, L. Parihar, Advancements in techniques used for identification of pesticide residue on crops, *J. Nat. Pestic. Res.* 4 (2023) 100031.
- [8] C.A. Damalas, S.D. Koutroubas, Farmers' exposure to pesticides: toxicity types and ways of prevention, *Toxics* 4 (1) (2016) 1.
- [9] B.K. Park, S.H. Kwon, M.S. Yeom, K.S. Joo, M.J. Heo, Detection of pesticide residues and risk assessment from the local fruits and vegetables in Incheon, Korea, *Sci. Rep.* 12 (1) (2022) 9613.
- [10] S. Mostafalou, M. Abdollahi, Pesticides and human chronic diseases: evidences, mechanisms, and perspectives, *Toxicol. Appl. Pharmacol.* 268 (2) (2013) 157–177.
- [11] L.Y. Xu, A.M. Abd El-Aty, J.B. Eun, J.H. Shim, J. Zhao, X.M. Lei, S. Gao, Y.X. She, F. Jin, J. Wang, M.J. Jin, B.D. Hammock, Recent advances in rapid detection techniques for pesticide residue: a review, *J. Agric. Food Chem.* 70 (41) (2022) 13093–13117.
- [12] A.R. Mostafalou, M. Abdollahi, S.H. Hosseini, Nanosized graphene oxide as a stable and efficient adsorbent for pesticide removal from contaminated water, *Environ. Sci. Pollut. Res.* 32 (12) (2025) 34567–34578.
- [13] Z.W. Chen, J.G. Zhao, Z.H. Liu, X.L. Bai, W.J. Li, Z.F. Guan, M. Zhou, H.W. Zhu, Graphene-delivered insecticides against cotton bollworm, *Nanomaterials* 12 (16) (2022) 2731.
- [14] X.D. Gao, F.Y. Shi, F. Peng, X.J. Shi, C.H. Cheng, W.L. Hou, H.C. Xie, X.H. Lin, X.P. Wang, Formulation of nanopesticide with graphene oxide as the nanocarrier of pyrethroid pesticide and its application in spider mite control, *RSC Adv.* 11 (57) (2021) 36089–36097.
- [15] P.T. Hu, L. Zhu, F. Zheng, J.Y. Lai, H.H. Xu, J.L. Jia, Graphene oxide as a pesticide carrier for enhancing fungicide activity against *Magnaporthe oryzae*, *New J. Chem.* 45 (5) (2021) 2649–2658.
- [16] B. Anegebe, I.H. Ifijen, M. Maliki, I.E. Uwidia, A.I. Aigbodion, Graphene oxide synthesis and applications in emerging contaminant removal: a comprehensive review, *Environ. Sci. Eur.* 36 (1) (2024) 15.
- [17] Y.W. Zhu, S. Murali, W.W. Cai, X.S. Li, J.W. Suk, J.R. Potts, R.S. Ruoff, Graphene and graphene oxide: synthesis, properties, and applications, *Adv. Mater.* 22 (35) (2010) 3906–3924.
- [18] T.T. Lang, M.Y. Xiao, W.Y. Cen, Graphene-based metamaterial sensor for pesticide trace detection, *Biosensors* 13 (5) (2023) 560.
- [19] A. Loudiki, M. Azriouil, M. Matrouf, F. Laghrib, A. Farahi, S. Saqrane, M. Bakasse, S. Lahrich, M.A. El Mhammedi, Graphene-based electrode materials used for some pesticide's detection in food samples: a review, *Inorg. Chem. Commun.* 144 (2022) 109891.
- [20] R. Xue, T.F. Kang, L.P. Lu, S.Y. Cheng, Electrochemical sensor based on the graphene-nafion matrix for sensitive determination of organophosphorus pesticides, *Anal. Lett.* 46 (1) (2013) 131–141.
- [21] V. Dasriya, R. Joshi, S. Ranveer, V. Dhundale, N. Kumar, H.V. Raghu, Rapid detection of pesticide in milk, cereal and cereal based food and fruit juices using paper strip-based sensor, *Sci. Rep.* 11 (2021) 18855.
- [22] K. Kumari, M.B. Singh, N. Tomar, A. Kumar, V. Kumar, K.L. Dabodhia, P. Singh, Adsorption of pesticides using graphene oxide through computational and experimental approach, *J. Mol. Struct.* 1291 (2023) 136043.
- [23] E. Lampiri, P.L. Yap, P. Berillis, C.G. Athanassiou, D. Losic, Graphene powders as new contact nanopesticides: revealing key parameters on their insecticidal activity for stored product insects, *Chemosphere* 364 (2024) 143200.
- [24] H.X. Wang, B.C. Hu, Z.S. Gao, F.J. Zhang, J. Wang, Emerging role of graphene oxide as sorbent for pesticides adsorption: experimental observations analyzed by molecular modeling, *J. Mater. Sci. Technol.* 63 (2021) 192–202.
- [25] Y. Chong, Y.F. Ma, H. Shen, X.L. Tu, X. Zhou, J.Y. Xu, J.W. Dai, S.J. Fan, Z.J. Zhang, The *in vitro* and *in vivo* toxicity of graphene quantum dots, *Biomaterials* 35 (19) (2014) 5041–5048.
- [26] T.A. Tabish, C.J. Scotton, D.C. Ferguson, L.X. Lin, A. van der Veen, S. Lowry, M. Ali, F. Jabeeen, M. Ali, P.G. Winyard, S.W. Zhang, Biocompatibility and toxicity of graphene quantum dots for potential application in photodynamic therapy, *Nanomedicine* 13 (15) (2018) 1923–1937.
- [27] H.J. Sun, L. Wu, W.L. Wei, X.G. Qu, Recent advances in graphene quantum dots for sensing, *Mater. Today* 16 (11) (2013) 433–442.
- [28] M.X. Li, T. Chen, J.J. Gooding, J.Q. Liu, Review of carbon and graphene quantum dots for sensing, *ACS Sens.* 4 (7) (2019) 1732–1748.
- [29] C.L. Lekshmi, U.S. Swathy, K. Vijayan, H. Simimole, S. Sumalekshmy, Graphene quantum dots derived from honey and mangostin as sustainable materials to construct fluorescence turn-on molecular switches for pesticide detection, *ChemistrySelect* 8 (13) (2023) e202204869.
- [30] M.R. Mahajan, P.O. Patil, Design of zero-dimensional graphene quantum dots based nanostructures for the detection of organophosphorus pesticides in food and water: a review, *Inorg. Chem. Commun.* 144 (2022) 109883.
- [31] C. Sahub, J.L. Andrews, J.P. Smith, M.A. Mohamad Arif, B. Tomapatnagat, J.W. Steed, Enhancement of sensitivity for dichlorvos detection by a low-weight gelator based on bolaamphiphile amino acid derivatives decorated with a hybrid graphene quantum dot/enzyme/hydrogel, *Mater. Chem. Front.* 5 (18) (2021) 6850–6859.
- [32] H.W. Chu, B. Unnikrishnan, A. Anand, Y.W. Lin, C.C. Huang, Carbon quantum dots for the detection of antibiotics and pesticides, *J. Food Drug Anal.* 28 (4) (2020) 539–557.
- [33] P. Tadawattana, K. Kawashima, S. Sittivanichai, J. T-Thienprasert, T. Mori, P. Pongprayoon, Exploring the capabilities of nanosized graphene oxide as a pesticide nanosorbent: simulation studies, *ACS Omega* 10 (9) (2025) 8951–8959.
- [34] Y.X. Xie, J. Zhao, X.Y. Li, J. Sun, H.F. Yang, Effects of cyfluthrin exposure on neurobehaviour, hippocampal tissue and synaptic plasticity in wistar rats, *Toxics* 11 (12) (2023) 999.
- [35] A. Wijewickrema, H. Banneheke, A. Pathmeswaran, F.W. Refai, M. Kaur-anaratne, N. Malavige, C. Jeewandara, M. Ekanayake, D. Samaraweera, D. Thambavita, P. Galappaththi, Efficacy and safety of oral ivermectin in the treatment of mild to moderate Covid-19 patients: a multi-centre double-blind randomized controlled clinical trial, *BMC Infect. Dis.* 24 (1) (2024) 719.
- [36] X.Z. Wu, J.Y. Li, Z. Zhou, Z.Q. Lin, S.M. Pang, P. Bhatt, S. Mishra, S.H. Chen, Environmental occurrence, toxicity concerns, and degradation of diazinon using a microbial system, *Front. Microbiol.* 12 (2021) 717286.
- [37] M. Galadima, S. Singh, A. Pawar, S. Khasnabis, D.S. Dhanjal, A.G. Anil, P. Rai, P. C. Ramamurthy, J. Singh, Toxicity, microbial degradation and analytical detection of pyrethroids: a review, *Environ. Adv.* 5 (2021) 100105.

- [38] Y. Yang, X.R. Zhang, J.Y. Jiang, J.R. Han, W.X. Li, X.Y. Li, K.M. Yee Leung, S.A. Snyder, P.J.J. Alvarez, Which micropollutants in water environments deserve more attention globally, *Environ. Sci. Technol.* 56 (1) (2022) 13–29.
- [39] D.W. Boukhvalov, M.I. Katsnelson, Modeling of graphite oxide, *J. Am. Chem. Soc.* 130 (32) (2008) 10697–10701.
- [40] C.V. Gomez, E. Robalino, D. Haro, T. Tene, P. Escudero, A. Haro, J. Orbe, Structural and electronic properties of graphene oxide for different degree of Oxidation1, *Mater. Today Proc.* 3 (3) (2016) 796–802.
- [41] A. Lerf, H.Y. He, M. Forster, J. Klinowski, Structure of graphite oxide revisited, *J. Phys. Chem. B* 102 (23) (1998) 4477–4482.
- [42] A.C. Reynosa-Martínez, G.N. Tovar, W.R. Gallegos, H. Rodríguez-Meléndez, R. Torres-Cadena, G. Mondragón-Solórzano, J. Barroso-Flores, M.A. Alvarez-Lemus, V.G. Montalvo, E. López-Honorato, Effect of the degree of oxidation of graphene oxide on As(III) adsorption, *J. Hazard. Mater.* 384 (2020) 121440.
- [43] M. Yusuf, F.M. Elfghi, S.A. Zaidi, E.C. Abdullah, M. Ali Khan, Applications of graphene and its derivatives as an adsorbent for heavy metal and dye removal: a systematic and comprehensive overview, *RSC Adv.* 5 (62) (2015) 50392–50420.
- [44] J.F. Liu, Y. Luo, X.F. Jiang, G.J. Sun, S.J. Song, M.F. Yang, J. Shen, Enhanced and sustained pesticidal activity of a graphene-based pesticide delivery system against the diamondback moth *Plutella xylostella*, *Pest Manag. Sci.* 78 (12) (2022) 5358–5365.
- [45] N.A. Garcia, J.B. Awuah, C.Y. Zhao, F. Vuković, T.R. Walsh, Simulation-ready graphene oxide structures with hierarchical complexity: a modular tiling strategy, *2D Mater.* 10 (2) (2023) 025007.
- [46] M.J. Frisch, G.W.T. H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, G. Scalmani, V. Barone, G.A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A.V. Marañenich, J. Bloino, B.G. Janesko, R. Gomperts, B. Mennucci, H.P. Hratchian, J.V. Ortiz, A.F. Izmaylov, J.L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V.G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J.A. Montgomery Jr., J.E. Peralta, F. Ogliaro, M.J. Bearpark, J. J. Heyd, E.N. Brothers, K.N. Kudin, V.N. Staroverov, T.A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A.P. Rendell, J.C. Burant, S.S. Iyengar, J. Tomasi, M. Cossi, J.M. Millam, M. Klene, C. Adamo, R. Cammi, J.W. Ochterski, R.L. Martin, K. Morokuma, O. Farkas, J.B. Foresman, D.J. Fox, *Gaussian* 16, 2016.
- [47] D.A. Case, H.M.A., K. Belfon, I.Y. Ben-Shalom, J.T. Berryman, S.R. Brozell, F.S. Carvahol, D.S. Cerutti, T.E. Cheatham III, G.A. Cisneros, V.W.D. Cruzeiro, T.A. Darden, N. Forouzes, M. Ghazimirsaeed, G. Giambasu, T. Giese, M.K. Gilson, H. Gohlke, A.W. Goetz, J. Harris, Z. Huang, S. Izadi, S.A. Izmailov, K. Kasavajhala, M.C. Kaymak, I. Kolossv'ay, A. Kovalenko, T. Kurtzman, T.S. Lee, P. Li, Z. Li, C. Lin, J. Liu, T. Luchko, R. Luo, M. Machado, M. Manathunga, K.M. Merz, Y. Miao, O. Mikhailovskii, G. Monard, H. Nguyen, K.A. O'Hearn, A. Onufriev, F. Pan, S. Pantano, A. Rahnamoun, D.R. Roe, A. Roitberg, C. Sagui, S. Schott-Verdugo, A. Shajan, J. Shen, C.L. Simmerling, N.R. Skrynnikov, J. Smith, J. Swails, R.C. Walker, J. Wang, J. Wang, X. Wu, Y. Wu, Y. Xiong, Y. Xue, D.M. York, C. Zhao, Q. Zhu, P.A. Kollman, *Amber* 2020, University of California, San Francisco, 2020.
- [48] BIOVIA, Discovery Studio, Discovery Studio 2021, Dassault Systèmes, San Diego, 2021.
- [49] A.W. Sousa da Silva, W.F. Vranken, ACPYPE - AnteChamber PYthon parser interface, *BMC Res. Notes* 5 (2012) 367.
- [50] B.H. Paul Bauer, Erik Lindahl, GROMACS 2022, 2022.
- [51] T. Darden, D. York, L. Pedersen, Particle mesh Ewald: an $N \cdot \log(N)$ method for Ewald sums in large systems, *J. Chem. Phys.* 98 (12) (1993) 10089–10092.
- [52] B. Hess, H. Bekker, H.J.C. Berendsen, J.G.E.M. Fraaije, LINCS: a linear constraint solver for molecular simulations, *J. Comput. Chem.* 18 (12) (1997) 1463–1472.
- [53] G. Bussi, D. Donadio, M. Parrinello, Canonical sampling through velocity rescaling, *J. Chem. Phys.* 126 (2007) 014101.
- [54] W. Humphrey, A. Dalke, K. Schulten, VMD: visual molecular dynamics, *J. Mol. Graph.* 14 (1) (1996) 33–38.
- [55] M.S. Valdés-Tresanco, M.E. Valdés-Tresanco, P.A. Valiente, E. Moreno, gmx_MMPBSA: a new tool to perform end-state free energy calculations with GROMACS, *J. Chem. Theor. Comput.* 17 (10) (2021) 6281–6291.
- [56] R. Kumari, R. Kumar, A. Lynn, G_mmpbsa: a GROMACS tool for high-throughput MM-PBSA calculations, *J. Chem. Inf. Model.* 54 (7) (2014) 1951–1962.
- [57] V. Subasinghege Don, L. Kim, R. David, J.A. Nauman, R. Kumar, Adsorption studies at the graphene oxide-liquid interface: a molecular dynamics study, *J. Phys. Chem. C Nanomater. Interfaces* 127 (12) (2023) 5920–5930.
- [58] P. Bolibok, S. Koter, A. Kaczmarek-Kędziera, P. Kowalczyk, B. Łukomska, O. Łukomska, S. Boncel, M. Wiśniewski, K. Kaneko, A.P. Terzyk, Liquid phase adsorption induced nanosizing of graphene oxide, *Carbon* 183 (2021) 948–957.
- [59] A. Molla, Y.Y. Li, B. Mandal, S.G. Kang, S.H. Hur, J.S. Chung, Selective adsorption of organic dyes on graphene oxide: theoretical and experimental analysis, *Appl. Surf. Sci.* 464 (2019) 170–177.
- [60] F. Moriggi, V. Barbera, M. Galimberti, G. Raffaini, Adsorption affinities of small volatile organic molecules on graphene surfaces for novel nanofiller design: a DFT study, *Molecules* 28 (22) (2023) 7633.
- [61] Q.Z. Jia, C. Yang, B.J. Venton, K.H. DuBay, Atomistic simulations of dopamine diffusion dynamics on a pristine graphene surface, *ChemPhysChem* 23 (4) (2022) e202100783.
- [62] M. Alonso, T. Woller, F.J. Martín-Martínez, J. Contreras-García, P. Geerlings, F. De Proft, Understanding the fundamental role of π/π , σ/σ , and σ/π dispersion interactions in shaping carbon-based materials, *Chem* 20 (17) (2014) 4845.
- [63] C. Janiak, A critical account on π - π stacking in metal complexes with aromatic nitrogen-containing ligands, *J. Chem. Soc. Dalton Trans.* 21 (2000) 3885–3896.
- [64] S. Yadav, A.P. Singh Raman, H. Meena, A.G. Goswami, Bhawna, V. Kumar, P. Jain, G. Kumar, M. Sagar, D.K. Rana, I. Bahadur, P. Singh, An update on graphene oxide: applications and toxicity, *ACS Omega* 7 (40) (2022) 35387–35445.
- [65] T. Jiang, C.A. Amadei, Y.S. Lin, N. Gou, S.M. Rahman, J.Q. Lan, C.D. Vecitis, A.Z. Gu, Dependence of graphene oxide (GO) toxicity on oxidation level, elemental composition, and size, *Int. J. Mol. Sci.* 22 (19) (2021) 10578.