

## AI-Integrated Chemistry Solutions for Sustainable Plastic Waste Management

<sup>a</sup>Enebi Estella Jasper, <sup>b</sup>Oteiva Mokie Frank, <sup>c</sup>Jude Chinedu Onwuka, and <sup>d</sup>Adeiza Jesse Omeiza

<sup>a</sup>Department of Chemical Sciences, Dennis Osadebay University, Asaba, Delta State.

<sup>b</sup>QAQC Department, INDORAMA-Elеме Petrochemicals Ltd, Port-Harcourt, Rivers State.

<sup>c</sup>Department of Science Lab. Tech, Federal University of Lafia, Nasarawa State.

<sup>d</sup>Department of Chemistry, Federal University of Lafia, Nasarawa State.

Corresponding Author's email: [enebi.jasper@dou.edu.ng](mailto:enebi.jasper@dou.edu.ng)

### ABSTRACT

One of the biggest environmental problems of the 21<sup>st</sup> century is plastic pollution. In order to handle the increasing amounts of plastic waste, traditional recycling and waste management techniques are frequently ineffective and insufficient. Artificial Intelligence (AI) has recently become an essential tool for enhancing recycling effectiveness, managing plastic waste, and creating sustainable plastic substitutes. With an emphasis on AI-enhanced recycling procedures, the expansion of recycling technologies, and the creation of biodegradable plastic substitutes, this paper examines the current status of AI-driven chemistry solutions in plastic waste management. The practical uses of AI in this field are highlighted by real-world case studies, which further illustrate how AI has the potential to completely transform the plastic waste management sector.

**KEYWORDS:** Plastic pollution, Artificial Intelligence (AI), Recycling, Sustainable, Biodegradable

### 1. INTRODUCTION

Plastics have a significant impact on modern life due to their durability, affordability, and versatility. However, for most of these same reasons, they have become recalcitrant and environmentally persistent. Globally, over 450 million tonnes of plastic are produced annually, with less than ten percent being effectively recycled.<sup>1</sup> The rest is either incinerated, dumped in landfills, or spills into the environment, where it continues to persist, contaminating soil and water, threatening aquatic life, obstructing drainage, affecting human health, and causing a host of other negative consequences. Incineration and photodegradation of these plastics release toxic fumes into the air, with degradation products traveling along the food chain, contributing to bioaccumulation in humans and resulting in a variety of health issues, including cancer.<sup>2</sup>

Conventional recycling methods, such as mechanical and chemical recycling, are inadequate and have a number of drawbacks.<sup>3</sup> For instance, sorting errors and high operational costs characterize mechanical recycling, which is the most common method.<sup>5</sup> Mechanical sorting also often renders sorted plastics non-recyclable.<sup>5</sup> Chemical recycling methods, on the other hand, which offer an alternative by breaking plastics down to monomers through pyrolysis, polymerization, and solvolysis, usually require a lot of energy and are not economical on a small scale.<sup>6</sup> Additionally, it produces secondary waste that could be harmful to the environment. It is based on the drawbacks of these conventional methods that artificial intelligence (AI), is being explored as a sustainable method for addressing plastic pollution more effectively. There is a global need for innovative solutions to the problem of plastic pollution, especially as increasing production and use continue to outweigh recycling and upscaling, thereby translating into a steady increase in plastic waste.

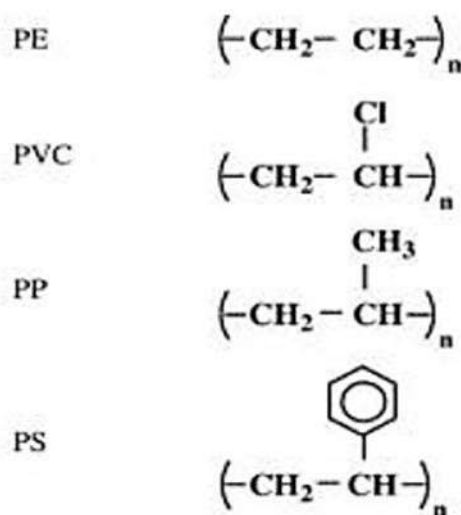
Artificial Intelligence (AI), with its ability to recognize patterns and make data-driven decisions, offers promising avenues for improving plastic waste management. When integrated with chemistry, AI can accelerate the design of sustainable materials, optimize degradation pathways, and transform recycling and policy systems. This review highlights the emerging integration of Artificial Intelligence (AI) with chemistry in tackling the global challenge of plastic pollution. Unlike conventional recycling-focused discussions, it further emphasizes AI-driven innovations in sustainable material design, optimization of plastic degradation pathways, and improvements in stages of waste management. It aims to provide a comprehensive synthesis of recent advances, identify knowledge gaps, and outline potential directions for future research. The scope encompasses AI applications in plastic detection, sorting, recycling, biodegradation, and sustainable alternatives, providing an all-

encompassing view of how AI and chemistry can transform global strategies for mitigating plastic pollution.

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## 2. THE CHEMISTRY OF PLASTIC WASTE

Plastic waste originates from synthetic polymers that are primarily derived from petrochemicals. Common examples, such as polyethylene (PE), polystyrene (PS), polypropylene (PP), and polyvinyl chloride (PVC) (Fig. 1), among others, are designed to be durable, hydrophobic, and chemically inert, which makes it difficult for them to degrade naturally.<sup>7</sup> When disposed of into the environment, these wastes are fragmented under UV radiation and mechanical stress, forming micro- and nanoplastics which retain the properties of the parent polymer.



**Fig 1: Common petrochemical-derived plastics (synthetic polymers) showing their repeating structural units**

These fragments persist in the ecosystem for several years, constituting a nuisance. Understanding the chemistry of plastic waste is crucial for determining its risks and for developing effective mitigation strategies to address plastic pollution. With advances in data analytics and computational chemistry, AI is being harnessed to transform the sorting, recycling, and redesigning of plastic waste for a sustainable future.

## 3. APPLICATIONS OF AI IN PLASTIC WASTE MANAGEMENT

AI provides powerful tools for addressing inefficiencies in the plastic waste lifecycle. Innovative AI-driven applications have been incorporated into critical stages of plastic pollution management, including sorting, recycling, and redesign. In sorting, AI-enabled robotic systems equipped with computer vision and sensor technologies have significantly improved the accuracy and speed of plastic classification. These systems analyze differences in color, composition, and shape in real time. AI-enabled robotic systems, such as those developed by AMP Robotics in the United States, use computer vision and deep learning to identify and sort different plastic types with high precision. The AMP Cortex system outperforms human workers by using deep learning to identify and sort up to 80 items per minute with over 95% accuracy.<sup>8</sup> A Finnish company, ZenRobotics, also uses AI-driven sorting to distinguish various polymer types using near-infrared spectroscopy (NIR), enhancing material recovery rates.<sup>9</sup> Systems like TOMRA's GAINnext™ combine hyperspectral imaging and convolutional neural networks (CNNs) to distinguish between polymers such as polyethylene terephthalate (PET) and

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highdensity polyethylene (HDPE), facilitating more effective separation and cleaner recycling streams.<sup>10</sup> This level of sorting precision is vital for chemical recycling processes, where contamination can significantly hinder material recovery.

In the domain of recycling, AI has helped to optimize reaction processes such as pyrolysis and depolymerization by adjusting factors that influence these processes, thus resulting in improved yield and energy efficiency. For instance, AI models can dynamically control reactor conditions and simulate reaction mechanisms to maximize depolymerization output for plastics like PET and polystyrene.<sup>11</sup> Catalysts have also been designed using machine learning (ML) to predict structure-reactivity relationships in mixed polymer streams for deconstructing and upcycling plastic waste.<sup>12</sup> Notably, AI-guided computational modeling using ML was instrumental in engineering hydrolases to depolymerise polyethylene terephthalate (PET). This research by Lu *et al.*<sup>13</sup> overcomes the challenge of recycling multicolored mixed PET products. Samsara Eco, an Australian climate technology company, has also developed enzyme-based recycling methods that are capable of breaking down nylon 6 and PET for unlimited reuse, offering a potential breakthrough in circular plastics.<sup>14</sup> Likewise, BASF's ChemCycling project utilizes AI-driven simulations to optimize the chemical recycling of mixed plastic waste, ensuring high yield and minimal byproducts.<sup>15</sup>

Concerning the redesign of sustainable plastics, AI is driving transformation by streamlining the discovery and optimization of environmentally friendly plastics. Through powerful simulations and predictive modeling, AI facilitates the design of materials such as polyhydroxyalkanoates (PHAs), polylactic acid (PLA), and other biodegradable nanocomposites tailored for durability and end-of-life degradation<sup>16,17</sup>. Collaboration between government, academia, and industry has been central to accelerating these innovations. In the United States, the BOTTLE (Bio-Optimized Technologies to keep Thermoplastics out of Landfills and the Environment) Consortium, launched by the U.S. Department of Energy, exemplifies public-private partnerships that leverage AI in plastic redesign. Using machine learning, robotics, and enzyme modeling, BOTTLE designs innovative plastics that are easier to recycle, thereby promoting circularity and material recovery.<sup>18</sup> Industries such as Danimer Scientific use AI-guided fermentation analytics to boost microbial production of polyhydroxyalkanoates (PHAs)—bioplastics derived from renewable feedstocks such as canola oil.<sup>19</sup> These redesign innovations, driven by AI, highlight a clear pathway toward closed-loop plastic economies.

## 5. CHALLENGES, LIMITATIONS, AND ETHICAL CONSIDERATIONS

Despite being a promising tool, AI's application to plastic waste management faces a lot of drawbacks, one of which is a lack of high-quality datasets on polymer behavior and properties. Model interpretability is another challenge, as many AI systems function as "black boxes," making predictions without offering precise justifications. This makes regulatory approval more difficult and diminishes stakeholder trust.<sup>20</sup> Furthermore, its use in low-income countries is limited by the poor distribution of technological infrastructure and a lower level of AI literacy.<sup>21,22</sup> Ethical concerns such as the risk of displacing human workers through automation, biases in training data, and the environmental costs of AI itself, particularly the energy demands of large-scale deep learning models, need to be taken into consideration.

## 6. CONCLUSION AND FUTURE DIRECTIONS

Plastic waste pollution presents one of the most persistent environmental crises of our time, threatening ecosystems, human health, and the sustainability of global development. Traditional waste management approaches have proven insufficient in mitigating the scale and complexity of plastic pollution. However, the integration of Artificial Intelligence and chemistry holds immense promise for transforming plastic waste from an environmental burden into a resource for innovation. By enabling smarter material design, real-time waste tracking, and optimized recycling processes, AI enhances the capabilities of chemistry in addressing one of the most pressing sustainability challenges of our time. However, realizing this potential requires addressing data, infrastructure, and ethical constraints through inclusive and interdisciplinary collaboration. With sustained investment and coordinated action, AI-integrated chemistry can catalyze a shift toward a more circular and sustainable plastics economy.

## CONFLICT OF INTERESTS

The authors declare no conflict of interest.

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