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Removal of heavy metals by polymers from wastewater in the industry: A molecular dynamics approach

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ABSTRACT

One of the major pollutants of industrial water is lead metal, which causes widespread pollution in nature due to its wide use. Removing this pollutant, before the surface or subsurface disposal of wastewater, is a very effective measure in preserving and preventing the pollution of natural resources and the environment. Since surface adsorption is one of the effective methods for removing waste materials from wastewater. This study utilized molecular dynamics simulation to investigate the interactions between lead and polypropylene (PP). PP has proven to be the most effective substance for eliminating lead from aquatic environments. Given the presence of heavy metals such as lead (Pb), cadmium (Cd), mercury (Hg), chromium (Cr), zinc (Zn), and nickel (Ni) in aquatic ecosystems, it becomes crucial to remove lead from the wastewater generated by the oil and petrochemical industries. The findings of this research have the potential to assist in the removal of lead from industrial wastewater settings.

1. Introduction

The world is facing a series of environmental crises, many of which are irreparable or if they are repaired, they are very expensive. Whenever living organisms are required to consume water, they inherently produce wastewater. This similarity can be observed in urban areas where approximately 75 to 80% of water consumption results in wastewater. Similarly, industries generate a proportionate volume of industrial wastewater [1–4]. Regrettably, the rapid advancement of industries, accompanied by the use of various new chemical compounds, has contributed to the accumulation of substantial quantities of industrial wastewater. Consequently, this has resulted in severe environmental contamination, particularly in water streams. Investigations show the fact that a large part of environmental crises and problems are the result of a series of policies and excessive exploitation of natural and environmental resources and the discharge of various pollutants caused by human activities in the environment and ultimately the lack of calculation The real value of environmental resources and costs of environmental destruction is in macroeconomic policies. Although the water resources available on the planet are significant, the resources that can be made available to humans are few, and for this reason, preventing possible pollution can help to a large extent to preserve the available water resources [5–7]. Many economists have come to believe that if the world community wants to use resources optimally, it must place environmental resources in the ranks of other scarce resources, and the economic rationality that governs the use of other production inputs, in the case of natural resources. And the environment should also be governed [8,9]. Industrial wastewater treatment is one of the topics that has been highly colored in recent years due to the reduction of water resources and the expansion of various industries. Because industries generally use a lot of water in their production operations. Also, due to the fact that some of this water is contaminated in the production process, it needs to be purified before being discharged and released into the environment. For this reason and due to the reduction of adverse environmental effects due to the discharge of industrial wastes, strict environmental laws have been applied by the country's environmental organization to the industrial effluents, in which the level of purification must protect the quality of water has been determined [10–12].

The development of various industries requires the design and implementation of all types of wastewater treatment packages, and without them, water treatment and industrial effluents cannot be performed properly. If the microbiological pollution of urban sewage can be

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INTRODUCTION

- Addresses the urgent need to remove lead from wastewater.
- Polypropylene (PP) is investigated as a potential adsorbent for lead removal.
- Explores the spatial distribution, conformational changes, and energy landscape of polymers at different concentrations.
- Findings provide insights for the design and optimization of polymer-based materials for industrial applications.

OBJECTIVE

- Investigate PP's effectiveness in removing lead from industrial wastewater.
- Analyze the spatial distribution and conformational changes of polymers during lead adsorption.
- Provide insights for optimizing polymer based materials for efficient lead removal.

METHODOLOGY

- Molecular dynamics(MD) simulations performed with PP polymer concentrations of 10, 15, 20, and 25, respectively.
- The simulations were conducted using the LAMMPS software.
- The structural and energetic properties of the polymer systems were analyzed using various techniques.

1. Gyration Radius analysis
2. RMSD analysis
3. RMSF analysis
4. SASA analysis

FORMULAS

$$R_g = \sqrt{\frac{\sum_i^N (r_i - \langle r_{com} \rangle)^2}{N}}$$

$$RMSF_i = \sqrt{\frac{\sum_J^M (r_{ij} - \langle r_i \rangle)^2}{M}}$$

$$RMSD_i = \sqrt{\frac{\sum_i^N (r_i - \langle r'_i \rangle)^2}{N}}$$

$$F = m \times a$$

$$F_{ij} = \frac{-dU_{(r)}}{dr}$$

$$E = \frac{1}{2} \times m \times v^2$$

$$F = -\nabla U$$

$$a = \frac{F}{m}$$

$$v = \frac{dx}{dt}$$

$$r = \sqrt{x^2 + y^2 + z^2}$$

RESULT & DISCUSSION

- The gyration radius exhibited temporal variations for all polymer concentrations examined over time based on the analysis.
- Differences were observed between the initial and final gyration radii values.

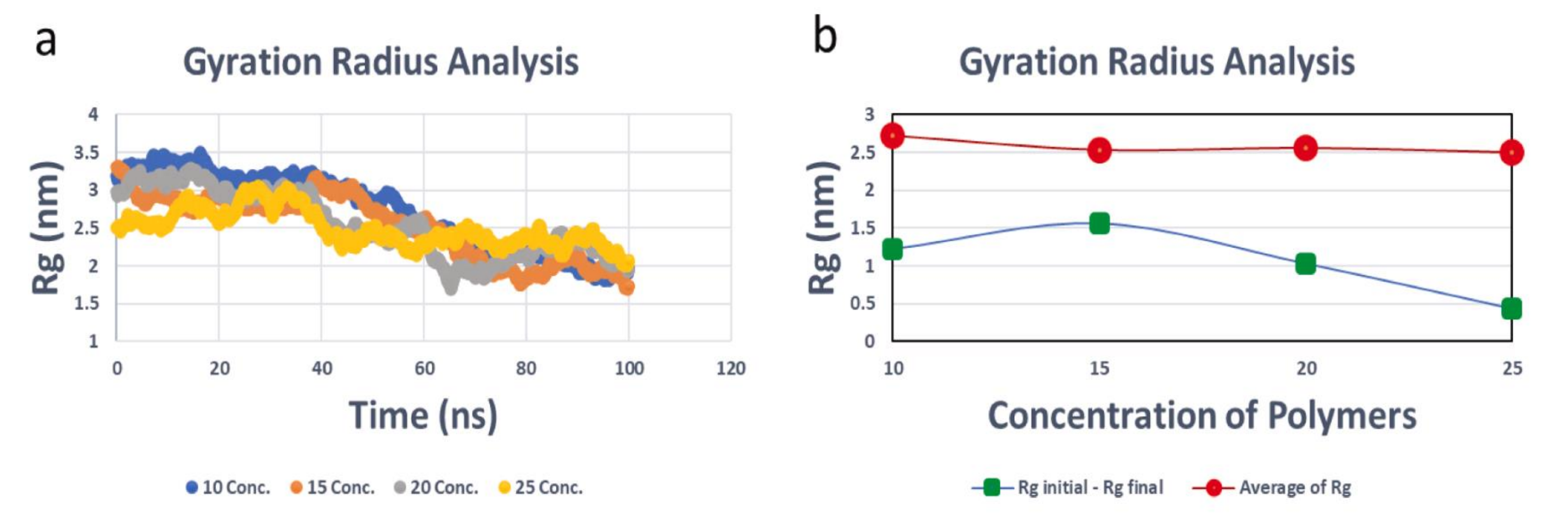
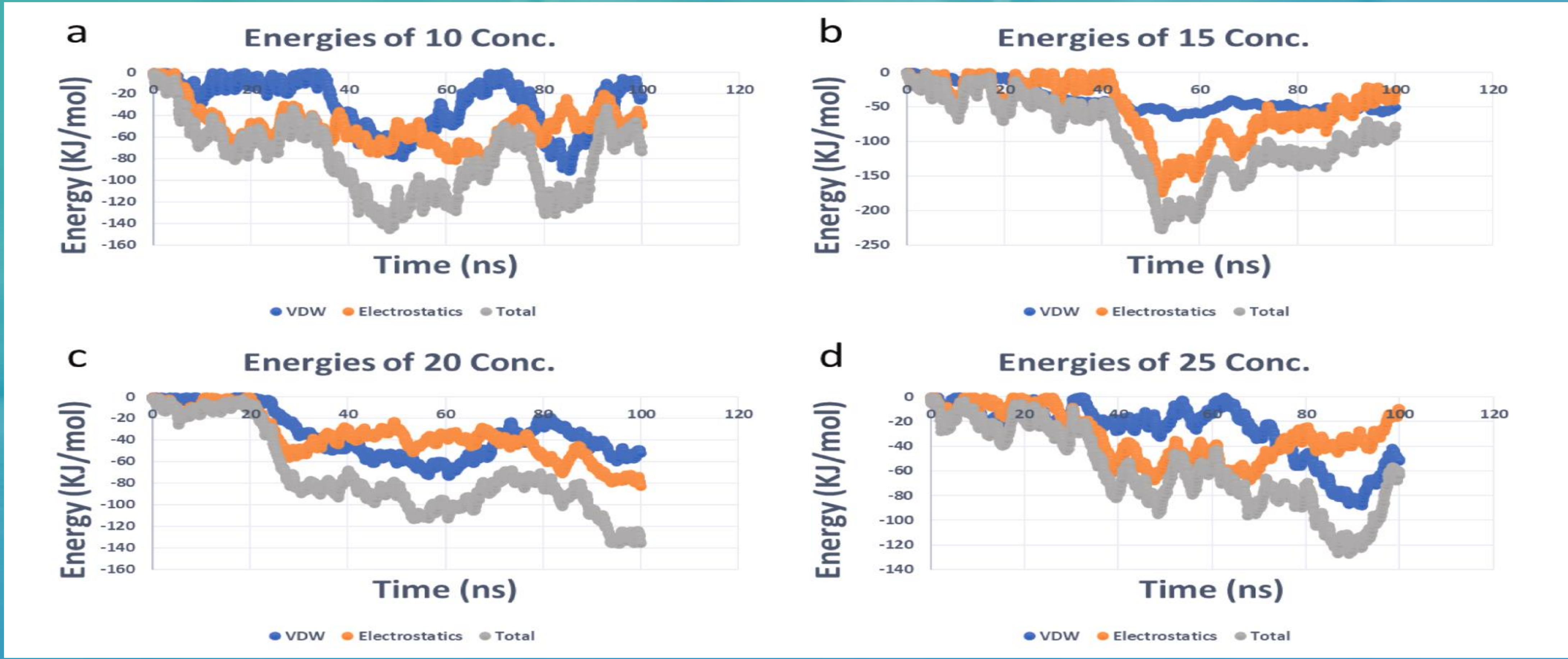


Chart a is time-dependent Rg analysis for different simulations.

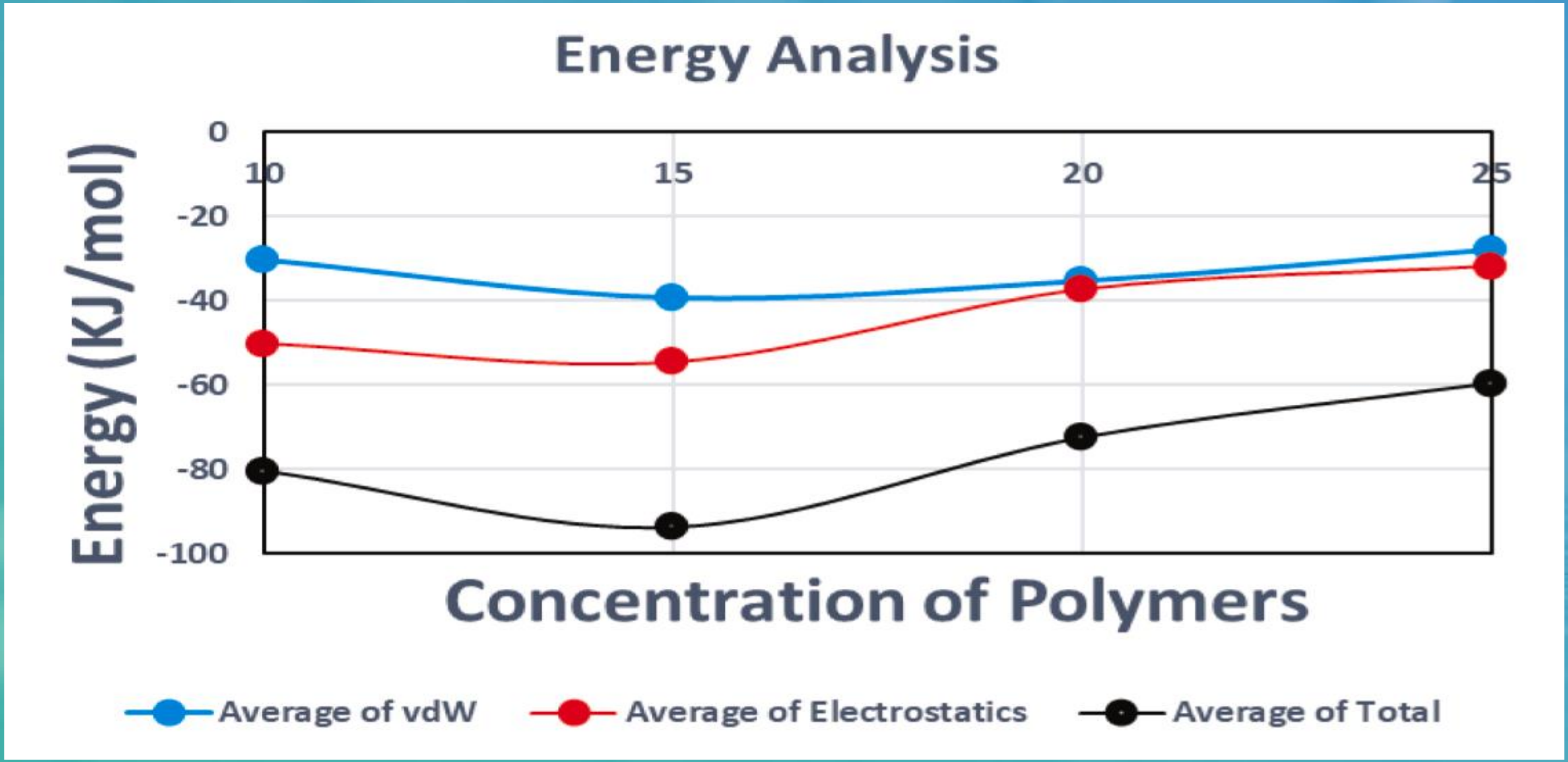
Chart b is differential of the initial and final Rg and the average Rg for the simulations.

- Average energy values vary significantly depending on polymer concentration, with concentration 15 showing the most favorable energies followed by 10, 20 and 25.
- Average energy values in the system were dependent on both VDW and electrostatic contributions, though VDW was more dominant for most concentrations.



Time-dependent analysis of and electrostatic and van der Waals (VDW) energies, as well as the total, for various concentrations.

- Polymer concentration 15 exhibited the lowest energy values over time based on analysis of electrostatic, VDW and total energies, with concentrations 10, 20 and 25 following closely behind.



Average analysis of electrostatic, total, and van der Waals (VDW) energies. Blue bar: average VDW energy, Red bar: average electrostatic energy, Black bar: average total energy.

- RMSD values varied over time for all concentrations but reached a plateau, indicating stable conformations were achieved.
- Concentration 15 had lowest average RMSD values, followed by 10, 20, 25 indicating better structural stability.

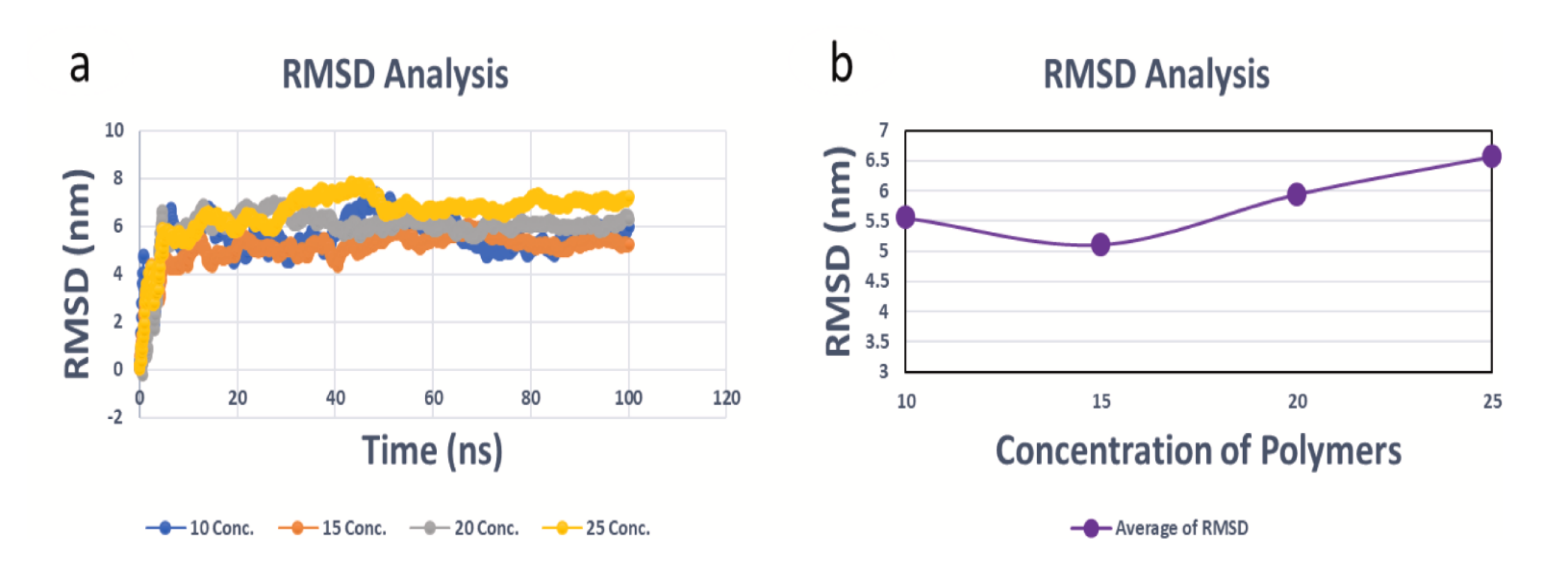
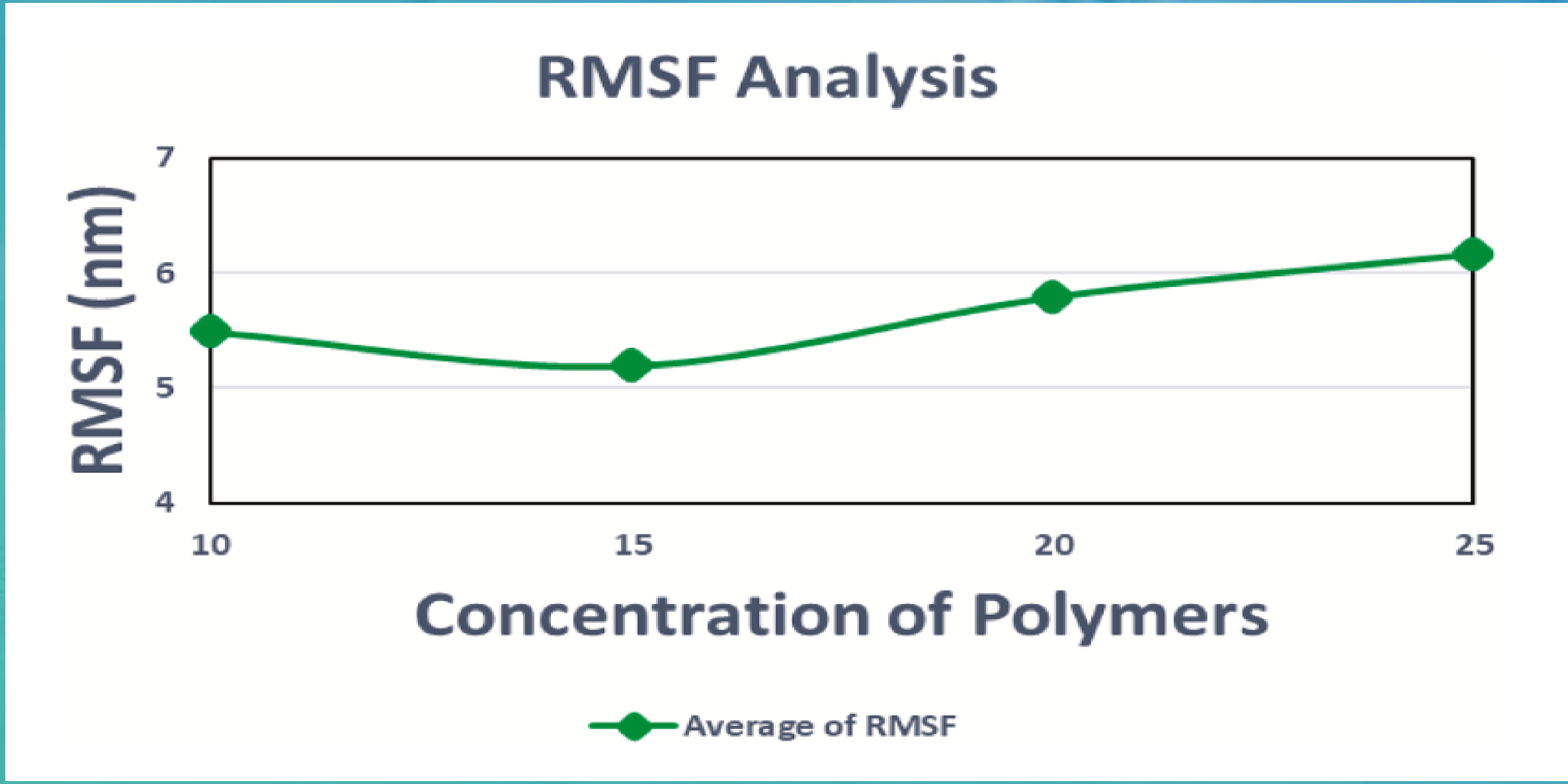


Chart a: time-dependent analysis of root-mean-square deviation (RMSD) for different polymer concentrations.

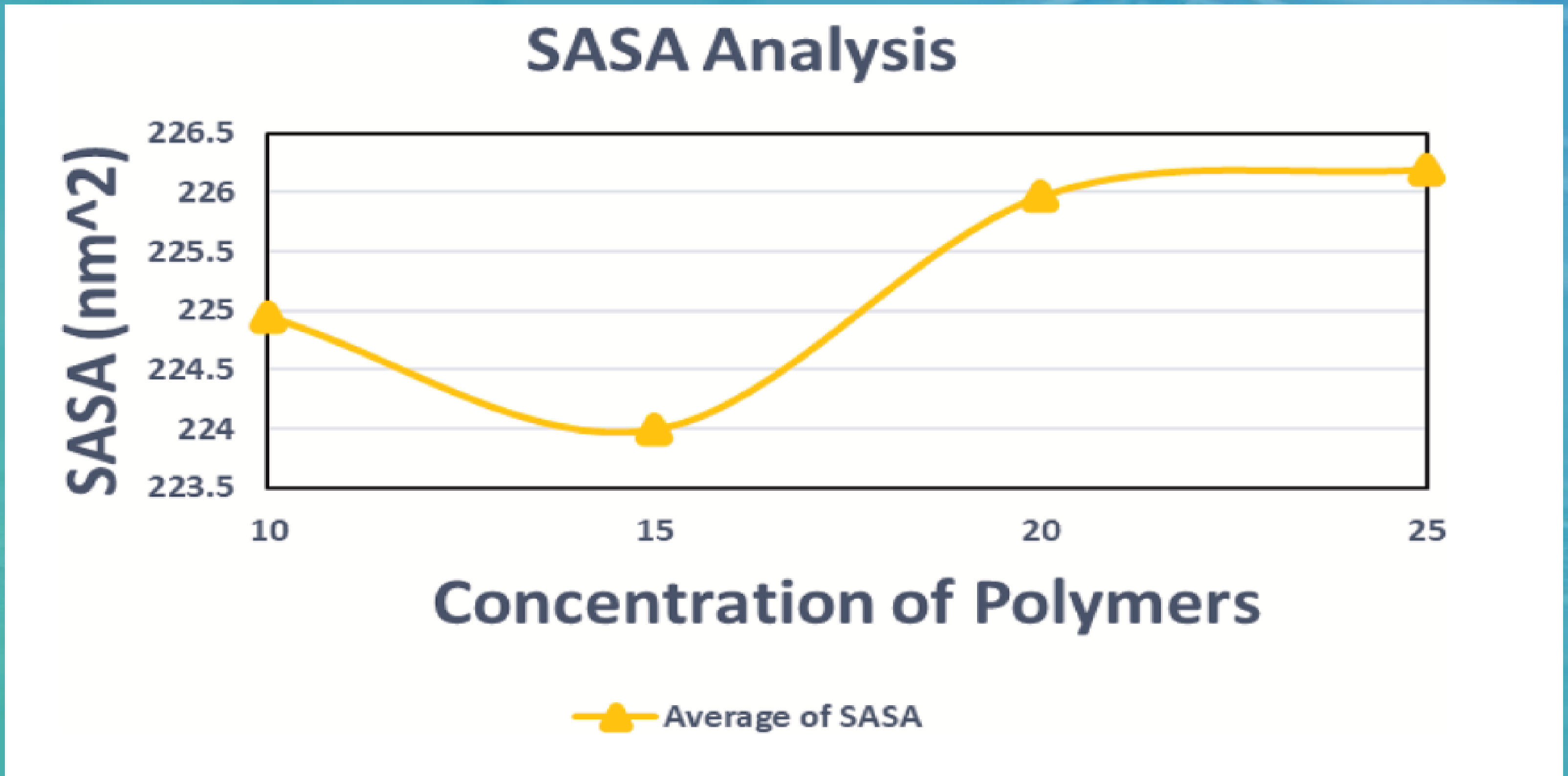
Chart b: average RMSD analysis.

- Polymer concentration 15 had the lowest average RMSF values, indicating a more stable system structure.
- Backbone fluctuations dominated most concentrations, but side-chain fluctuations increased at higher concentrations.



Average analysis of RMSF for different polymer concentrations in the simulations.

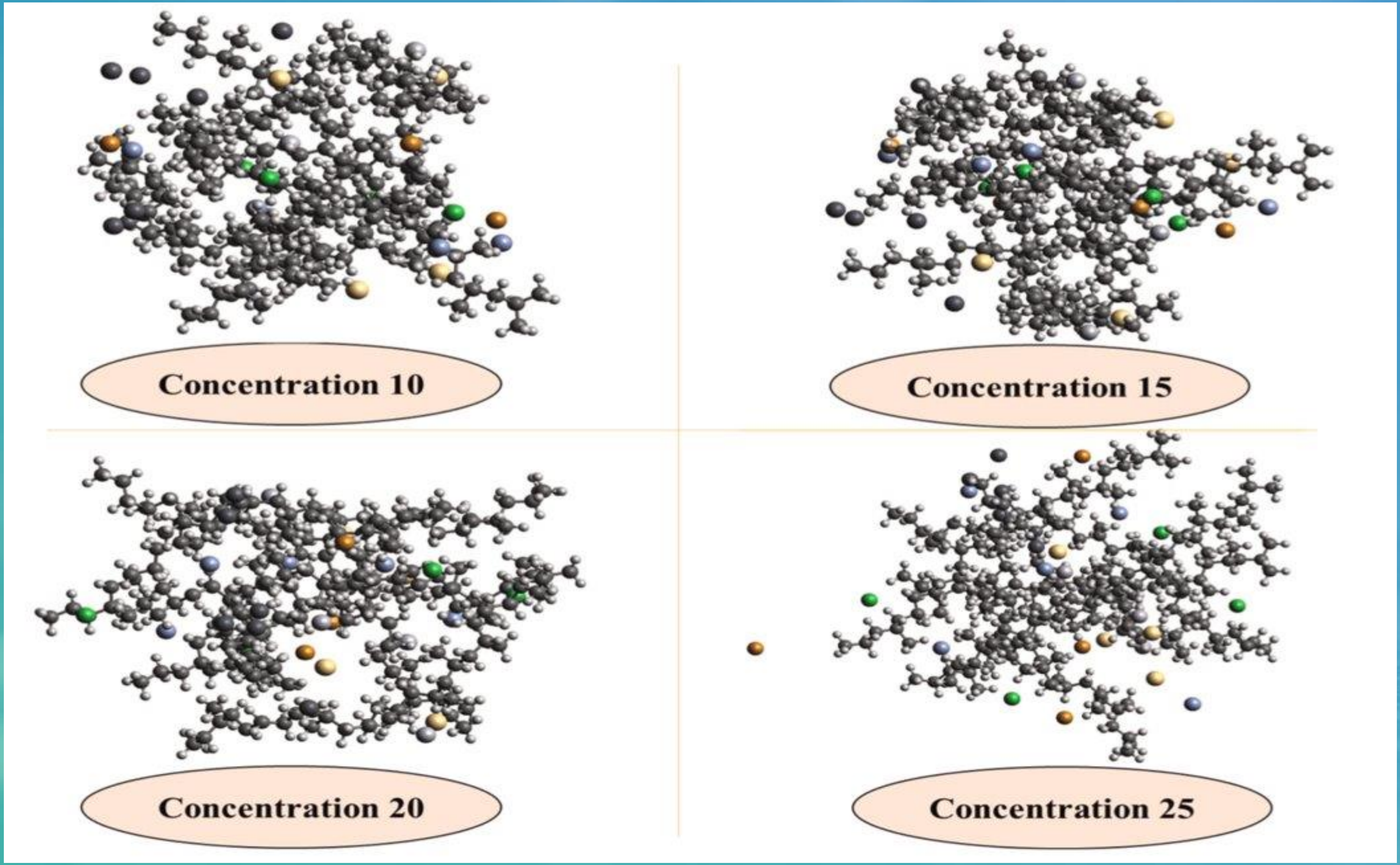
- Polymer concentration of 15 had the lowest average SASA values, indicating the most compact surface area.
- Visual analysis showed concentration 15 formed the most tightly packed and ordered final structure compared to other concentrations.



Average analysis of solvent-accessible surface area (SASA) for different polymer concentrations in the simulations.

CONCLUSION

- ✓ Polypropylene effectively adsorbs lead atoms from wastewater streams.
- ✓ Molecular dynamics simulations show polypropylene remains stable when removing lead in water environments.
- ✓ Polypropylene proves to be an optimal material for removing lead from petrochemical plant effluents.
- ✓ This research enables practical and safe application of polypropylene for lead removal in the oil and petrochemical industries.



Final frame of simulations at the different concentrations. Polymer is PP and heavy metals include Lead (Pb), Mercury (Hg), Zinc (Zn), Chromium (Cr), Cadmium (Cd), and Nickel (Ni).

FUTURE WORK

- Simulate the adsorption of other heavy metals like cadmium, mercury, chromium etc. on PP polymer to evaluate its effectiveness in removing multiple pollutants from industrial wastewater.

- Conduct experiments to validate the results from molecular dynamics simulation of lead adsorption on PP. This will help in practical application of PP for industrial wastewater treatment.

- Study the effect of parameters like temperature, pressure, polymer chain length etc. on the adsorption mechanism and capacity. Optimizing these parameters can further enhance the pollutant removal efficiency.

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THANK YOU