Adsorption of Wastewater Pollutants on Lignocellulosic Biomass – a Molecular Dynamics Simulations Viewpoint

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Introduction

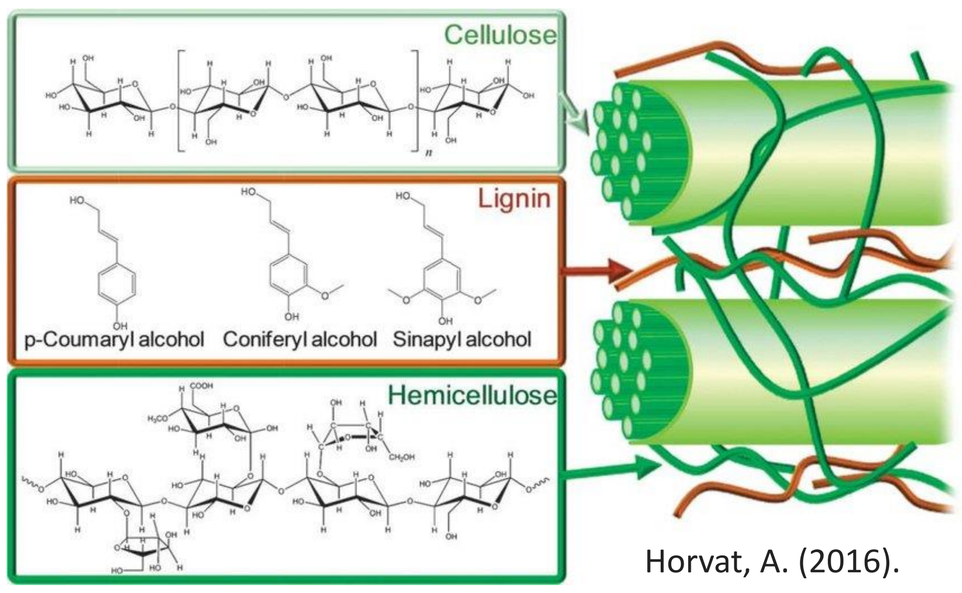
- Reducing the costs of water treatment is essential not only to increase the accessibility to water but also to encourage industries to reuse their liquid waste.
- Some lignocellulosic biomass such as the husk of coconuts, rice, and peanuts offer great potential for developing low-cost water treatment systems due to their high adsorption capacities and their availability as a waste, especially in tropical countries (Bhatnagar et al., 2010).
- The adsorption mechanism on lignocellulosic biomass is not well established in the literature, which limits its applicability in water treatment (James & Yadav, 2021).

Objective

This research project had the objective of using molecular dynamics simulations (GROMACS package) to study the adsorption mechanism of wastewater pollutants on lignocellulosic biomass. The project aimed to provide adsorption kinetic and thermodynamic data that could be used to optimize low-cost water treatment systems based on lignocellulosic agricultural waste such as coconut coir, rice husk, and peanut hull.

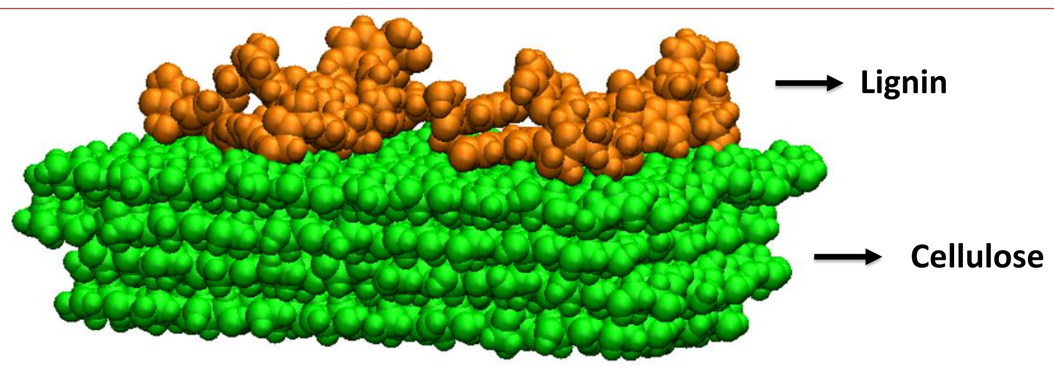
Study Design

Structure of Lignocellulosic Biomass:



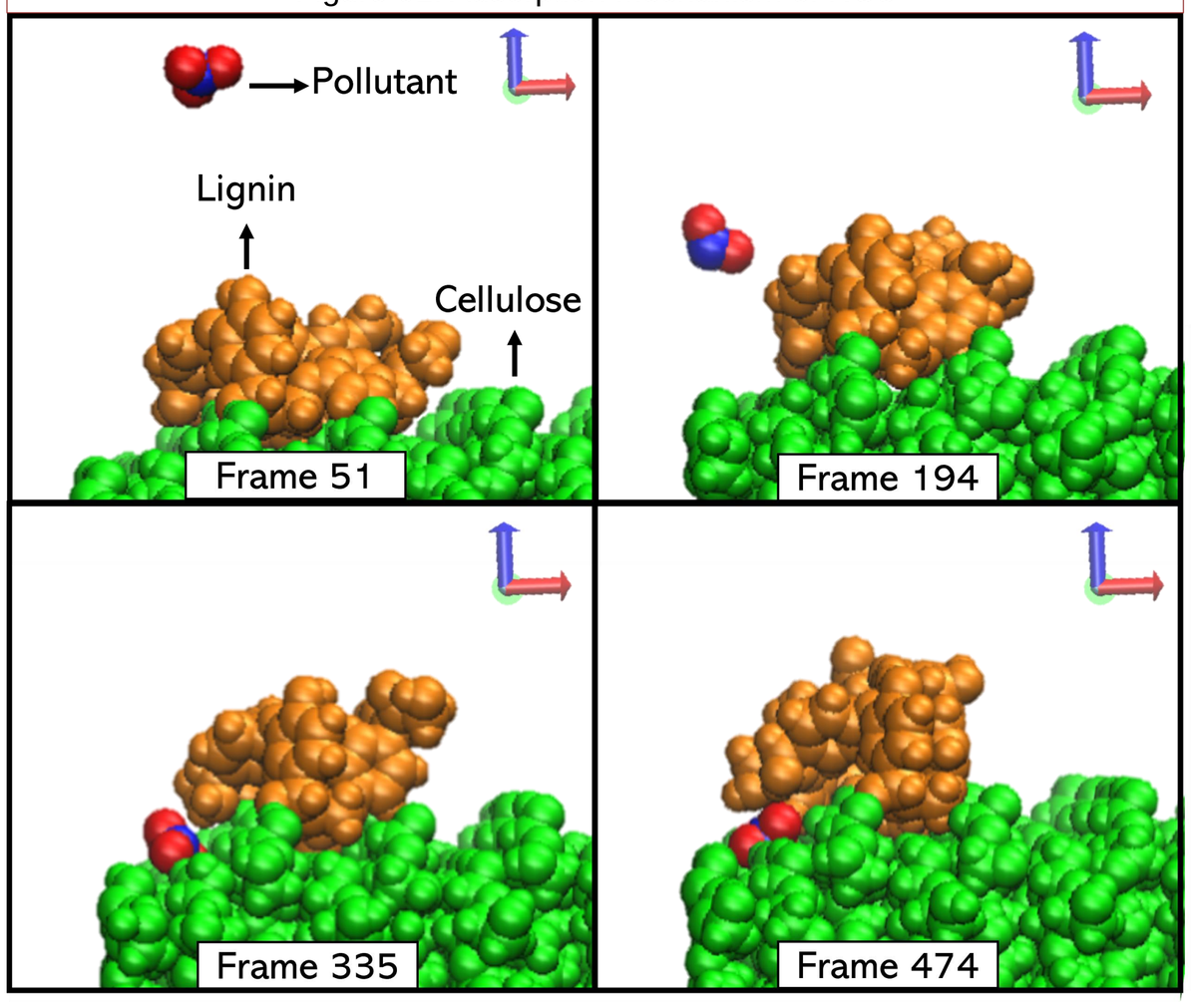
Horvat, A. (2016).

Our Model for Lignocellulosic Biomass:



Adsorption Mechanism

Figure 01: Adsorption Mechanism of NO3



Temperature Dependence of Adsorption

Figure 02: Temperature Dependence of Heavy Metal Adsorption

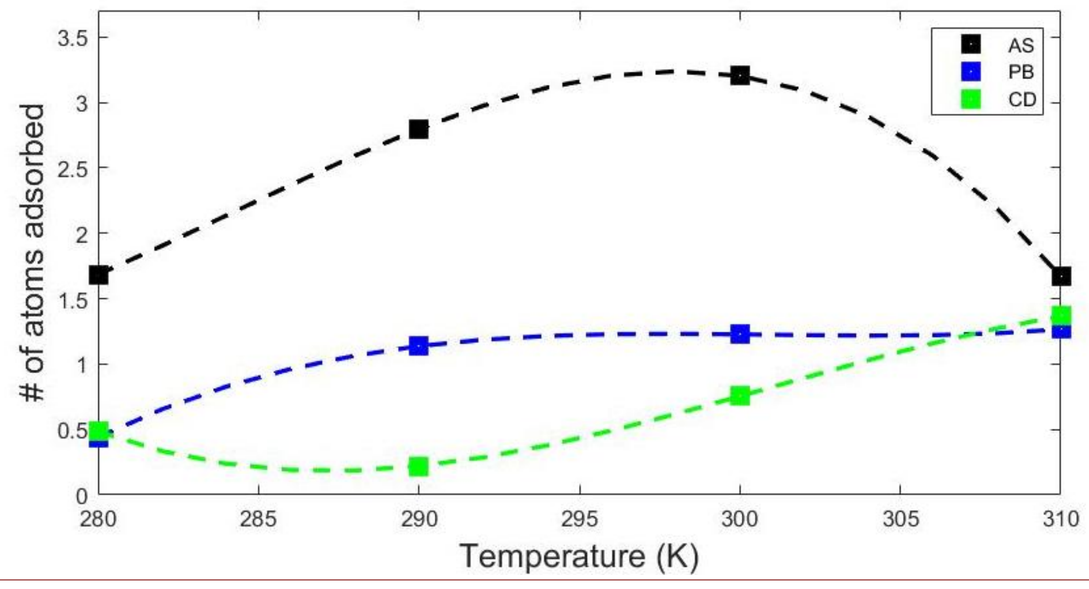
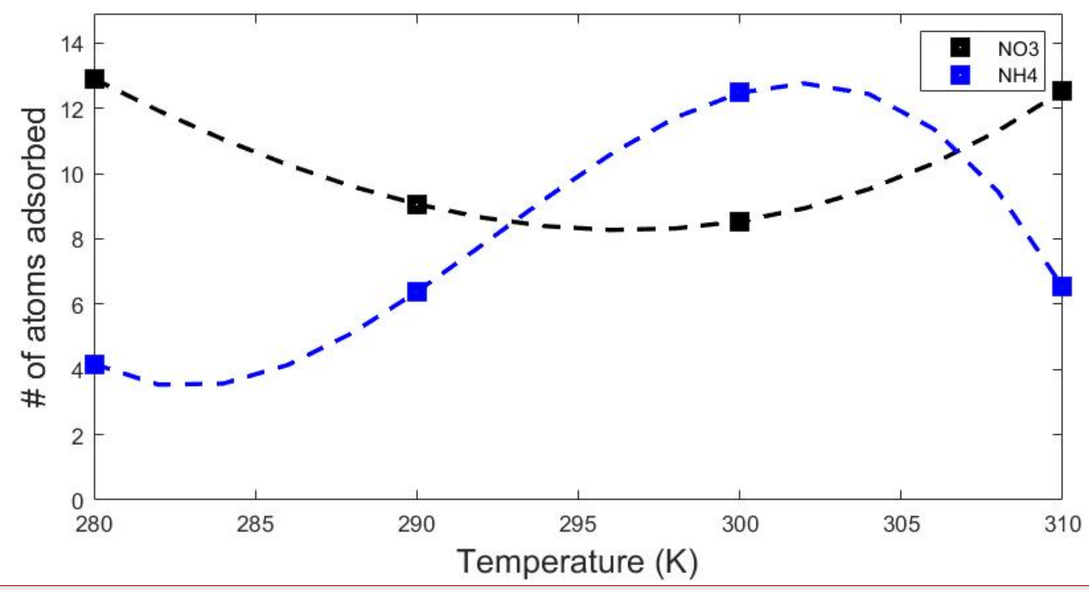
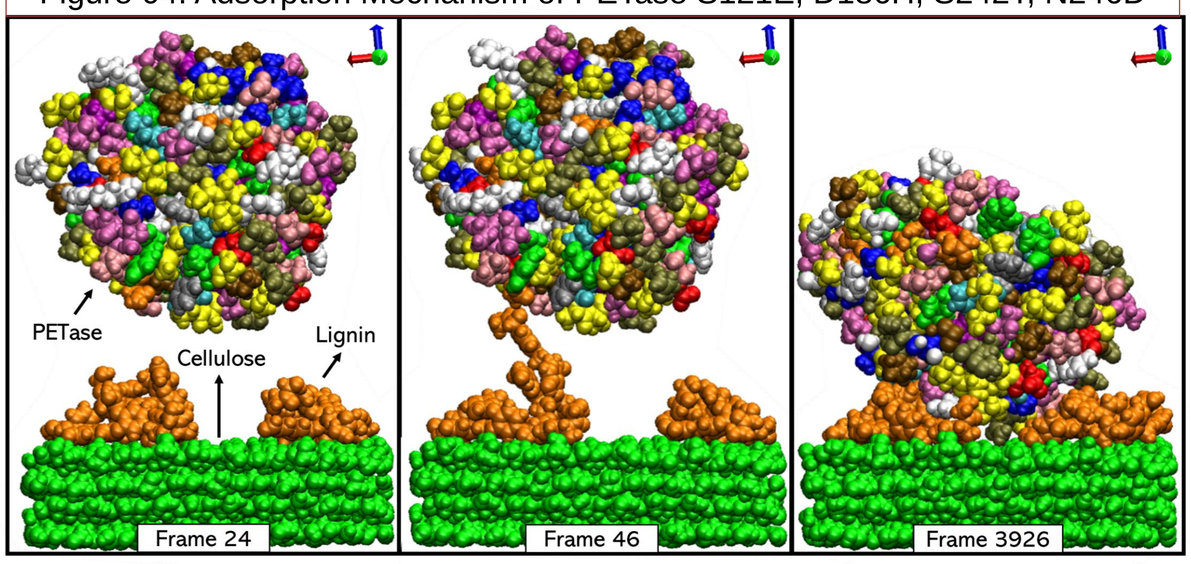


Figure 03: Temperature Dependence of Nitrous Species Adsorption



Enzyme Adsorption

Figure 04: Adsorption Mechanism of PETase S121E, D186H, S242T, N246D



Conclusions

- The results evidence that in the adsorption mechanism of lignocellulosic biomass, cellulose forms stable electrostatic interactions with pollutants and lignin serves as a “molecule catcher”, attracting adsorbents, bringing them close to cellulose, then physically blocking their way out
- Temperature dependency simulations showed that for each pollutant there is an optimum temperature in which adsorption is maximized, being consistent with experimental data in the literature.
- Enzyme adsorption studies showed that lignocellulosic materials can form stable interactions with a PETase mutant, which could be used to develop low-cost systems to remove microplastics from water.

References

- Bhatnagar, A., Vilar, V. J., Botelho, C. M., & Boaventura, R. A. (2010). Coconut-based biosorbents for water treatment—a review of the recent literature. Advances in colloid and interface science, 160(1-2), 1-15.
- Horvat, A. (2016). A study of the uncertainty associated with tar measurement and an investigation of tar evolution and composition during the air-blown fluidised bed gasification of torrefied and non-torrefied grassy biomass..
- James, A., & Yadav, D. (2021). Valorization of coconut waste for facile treatment of contaminated water: A comprehensive review (2010–2021). Environmental Technology & Innovation, 24, 102075.