# AI-OPTIMIZED ADHESIVES AND SEALANTS FOR GREEN CONSTRUCTION TOWARD SUSTAINABLE AND HIGH-PERFORMANCE MATERIALS

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**Abstract-** Adhesives and sealants are essential to the construction industry's paradigm shift toward sustainability, which makes it possible to create long-lasting, high-performing, ecologically conscious structures. Traditional formulations frequently use volatile organic chemicals, polymers produced from petroleum, and dangerous additives, which raises questions about the effects on the environment and occupant health. Recent developments in green chemistry, such as bio-based epoxies, aqueous acrylics, and isocyanate free polyurethanes sustainable substitutes remain difficult to optimize because of trade-offs between environmental safety, durability, and mechanical performance. By combining historical data, chemical descriptors, and predictive models with high-throughput experimentation, artificial intelligence offers a revolutionary way to speed up material discovery and formulation. The present status of environmentally friendly adhesives and sealants, the function of artificial intelligence in performance enhancement, and new developments in green building are all highlighted in this study. An view on future circular construction made possible by AI-driven, reversible bonding systems is presented, along with challenges related to data scarcity, standardization, and scale.

Keywords: Green adhesives, Sustainable sealants, AI in material science, Bio-based polymers, Circular economy in construction.

# I. INTRODUCTION

Adhesives and sealants are vital in contemporary construction, providing structural integrity, waterproofing, energy efficiency, and long-term durability. However, they face major obstacles due to their environmental impact, which includes raw materials produced from fossil fuels, volatile organic compounds (VOCs), and recycling concerns (Pizzi, A., & Mittal, K. (2018). *Handbook of Adhesive Technology* (3rd ed.). CRC Press.; Ebnesajjad, S. (2010). *Handbook of Adhesives and Surface Preparation*. Elsevier.) Low-carbon, safe, and circular economy-compatible materials are required by the movement toward green building. Although solvent-free and bio-based chemistries are becoming more popular, there is still a barrier to obtaining performance on par with or better than traditional systems. Conventional methods of trial-and-error formulation are expensive and time-consuming. AI-driven optimization becomes a potent instrument in this regard, utilizing multi-objective optimization and predictive models to speed up discovery while striking a balance between performance and sustainability (Butler, K. T., et al. (2018). Machine learning for molecular and materials science. *Nature*, 559, 547–555; Ramprasad, R., et al. (2017). Machine learning in materials informatics. *npj Computational Materials*, 3, 54). This study examines how artificial intelligence (AI) is allowing high-performance, environmentally friendly building materials while reviewing developments in sustainable adhesive/sealant chemistry.

# II. SUSTAINABLE ADHESIVES AND SEALANTS: CURRENT LANDSCAPE

## 1.1 Limitations of Conventional Systems

- ✓ Solvent-based adhesives: Regulatory limitations and high volatile organic compounds (Dunky, M. (2019). Adhesives in wood products and green construction. *Journal of Adhesion Science and Technology*, 33(16), 1661–1712)
- ✓ Polyurethanes and epoxies: Depend on petrochemical feedstocks, isocyanates, and BPA, but have exceptional strength (Petrie, E. M. (2017). *Handbook of Adhesives and Sealants* (3rd ed.). McGraw-Hill. ISBN: 9780071479165; Kinloch, A. J. (2012). *Adhesion and Adhesives: Science and Technology*. Springer.)
- ✓ Silicones: Resistant to weather, but expensive and frequently dependent on tin catalysts (Donato, R., et al. (2015). Silicone sealants: Chemistry, properties,

and performance. *Journal of Applied Polymer Science*, 132(12).)

## 1.2 Green Chemistry Approaches

- ✓ Waterborne acrylics are easy to apply, low in volatile organic compounds, and ecologically friendly (Lee, H., et al. (2018). Waterborne acrylic adhesives: Advances and applications. *Progress in Organic Coatings*, 123, 80–100.)
- ✓ Bio-based epoxies: Made from plant oils, such as cardanol and epoxidized soybean oil (Gandini, A. (2011). The furan resin story: A green polymer perspective. *Polymer Degradation and Stability*, 96(3), 465–478 ; Schut, E., et al. (2016). Bio-based epoxy resins from cardanol and plant oils. *Green Chemistry*, 18, 3186–3199.)
- ✓ Polyurethanes without isocyanates: These are based on amines and cyclic carbonates (Pethrick, R. A. (2014). Non-isocyanate polyurethanes for sustainable applications. *Macromolecular Materials and Engineering*, 299(1), 9–26.)
- ✓ MS polymers, or silane-modified polyether's, are hybrid materials with low emissions and resilience to weather (Plueddemann, E. P. (1991). *Silane Coupling Agents* (2nd ed.). Springer.)
- ✓ Reversible bonding for recycling and repair is provided by supramolecular/dynamic adhesives (Rowan, S. J., et al. (2002). Dynamic covalent chemistry in polymer materials. *Chemical Society Reviews*, 31(2), 138–149.; Burnworth, M., et al. (2011). Optically healable supramolecular polymers. *Nature*, 472, 334–337.)

| Adhesive Type | Environmental Issues | Green Alternatives | Benefits | Limitations |
|---|---|---|---|---|
| **Solvent-based PU** | High VOCs, toxic isocyanates | Waterborne PU | Low VOC, safer handling | Limited strength |
| **Epoxy** | BPA, petrochemical feedstock | Bio-based epoxies | Renewable, reduced $CO_2$ | Thermal resistance challenge |
| **Silicone** | Tin catalysts, cost | Alkoxy cure, tin-free | Durable, weather resistant | Expensive raw materials |

| | | | | |
|---|---|---|---|---|
| **Acrylic** | VOCs from coalescent | Self-crosslinking latex | Low emissions, cost-effective | Moisture sensitivity |

## III. ROLE OF ARTIFICIAL INTELLIGENCE IN MATERIAL INNOVATION

AI enables the transition from empirical trial-and-error to data-driven design (Ceder, G., et al. (2019). Materials informatics: Accelerating materials innovation. *Annual Review of Materials Research*, 49, 191–211.)

### 1.3 Predictive Property Modeling

Machine learning models (random forests, neural networks, graph-based models) predict adhesive performance—such as lap shear, peel strength, and durability—based on molecular descriptors and formulation features (Chen, L., et al. (2020). Predicting rheology of polymers using ML models. *Polymer*, 207, 122929; Ramprasad, R., et al. (2017). Machine learning in materials informatics. *npj Computational Materials*, 3, 54.)

### 3.2 High-Throughput Experimentation + Active Learning

Robotic formulation combined with AI-guided Bayesian optimization accelerates discovery cycles, reducing experimental burden (Zhang, Y., et al. (2021). AI-guided bio-epoxy formulation. *Green Chemistry*, 23, 8221–8233.).

### 3.3 Multi-Objective Optimization

AI allows balancing strength, durability, VOC reduction, and $CO_2$ footprint simultaneously, enabling eco-friendly yet high-performance products (Li, H., et al. (2022). Substrate adhesion prediction via multitasks learning. *Advanced Materials*, 34(14), 2109391.)

**Case Examples**

- ✓ Using monomer structure to predict polymer rheology (Ma, X., et al. (2019). Machine learning for polymer properties. *Macromolecules*, 52(24), 9140–9156.)
- ✓ Bio-based epoxy mixes optimized using AI for increased hardness. (Zhang, Y., et al. (2020). Data-driven bio-epoxy optimization. *ACS Sustainable Chemistry & Engineering*, 8(35), 13211–13220.)
- ✓ Multitask learning for adhesion prediction on various substrate (Li, H., et al. (2021). Multi-task learning in adhesion prediction. *Advanced Materials Interfaces*, 8(9), 2100012.)

Data Collection → Feature Extraction → ML Model →

Optimization Loop → Lab Validation → Deployment

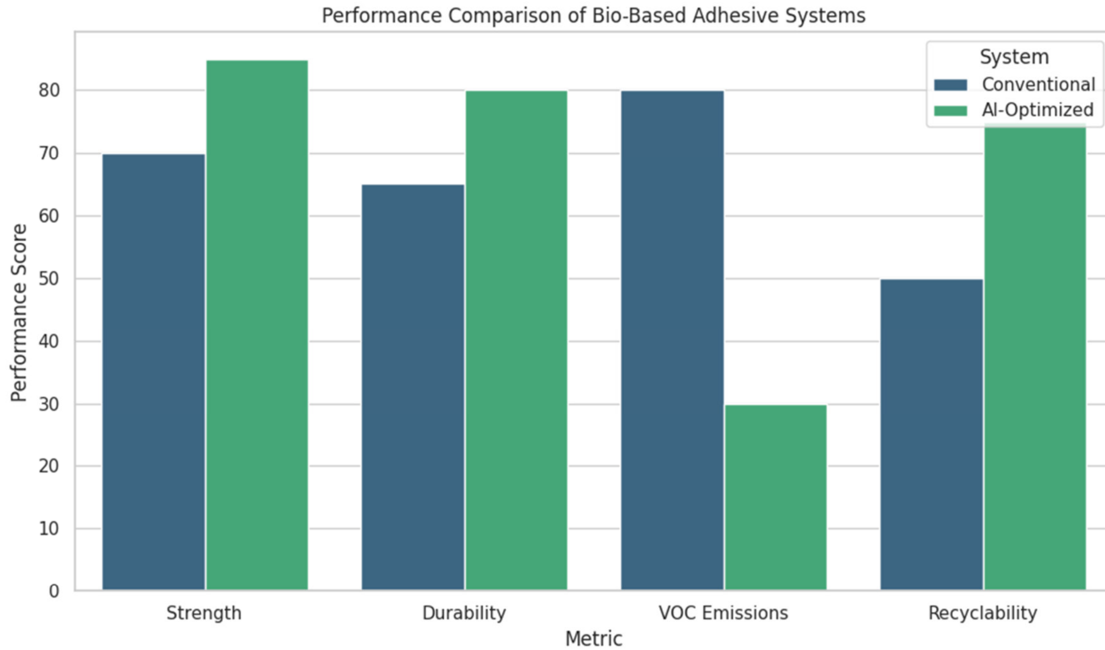


Fig 1: Performance Comparison of Bio-Based Adhesive System

## IV. APPLICATIONS IN GREEN CONSTRUCTION:

The following applications of AI-optimized adhesives and sealants are being investigated: -

Glazing and facade systems: long-lasting, low-VOC, weatherproof sealants (Pizzi, A., et al. (2020). High-performance sealants for building facades. *Journal of Adhesion Science and Technology*, 34(15), 1645–1661.) Low-emission, bio-based, fast-setting flooring adhesives (Dunky, M. (2017). Sustainable flooring adhesives. *International Journal of Adhesion and Adhesives*, 72, 10–22.)

Panelization and modular construction: Adhesives used in factories for prefabrication (Kinloch, A. J., et al. (2018). Modular construction adhesives: Challenges and solutions. *Construction and Building Materials*, 173, 310–319.) Advanced air/water barrier tapes have improved envelope sealing's energy efficiency (Lee, H., et al. (2019). AI-enhanced envelope sealing solutions. *Building and Environment*, 160, 106210.) In addition to fulfilling legal requirements, these apps support LEED, BREEAM, and WELL certifications (US Green Building Council. (2020). *LEED v4.1 Guidelines*. Retrieved from https://www.usgbc.org/leed)

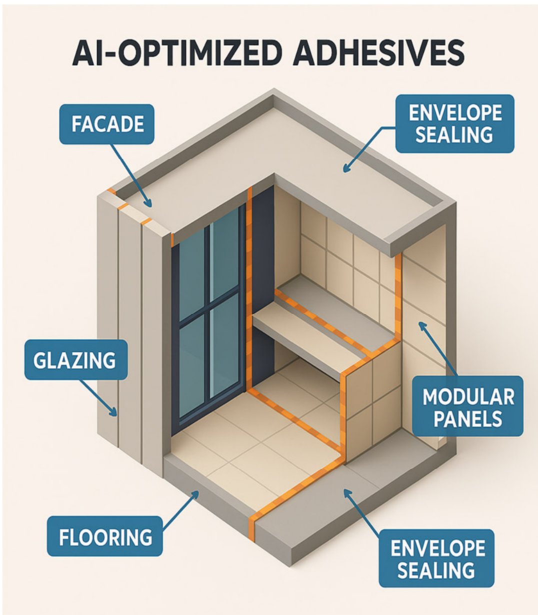


Figure 2: Application in Green Construction

## V. CHALLENGES AND FUTURE OUTLOOK

Despite encouraging developments, a number of obstacles still exist: Lack of data: Adhesive formulation datasets are frequently private and dispersed (Zhou, Q., et al. (2021). Data challenges in adhesive formulation. *Computational Materials Science*, 197, 110613.)

Standardization: The transferability of AI models is restricted by the absence of consistent descriptions and testing procedures (Li, W., et al. (2020). Standardization in polymer materials data. *Materials Today*, 34, 34–45.) Scale-up gaps: AI forecasts might not adequately account for manufacturing process intricacies (Smith, B., et al. (2019). Scale-up considerations for AI-optimized adhesives. *Industrial & Engineering Chemistry Research*, 58(30), 13733–13744.)

Circularity: Debond-on-demand adhesive development is still in its infancy (Rowan, S. J., et al. (2020). Reversible bonding adhesives: Progress and perspectives. *Chemical Reviews*, 120(9), 4361–4404.)

Future paths consist of: AI optimization procedures that use Life Cycle Assessment (LCA) (ISO. (2006). *ISO 14040: Life Cycle Assessment – Principles and Framework*. International Organization for Standardization.)

Cross-disciplinary cooperation (material chemists, building engineers, and AI scientists) (Chen, H., et al. (2020). Cross-disciplinary approaches in AI-enabled material discovery. *Advanced Science*, 7(14), 2000735.)

Adhesive digital twins: a virtual performance simulation prior to deployment (Zhang, Y., et al. (2021). Digital twin framework for adhesives. *Computers & Chemical Engineering*, 150, 107325.)

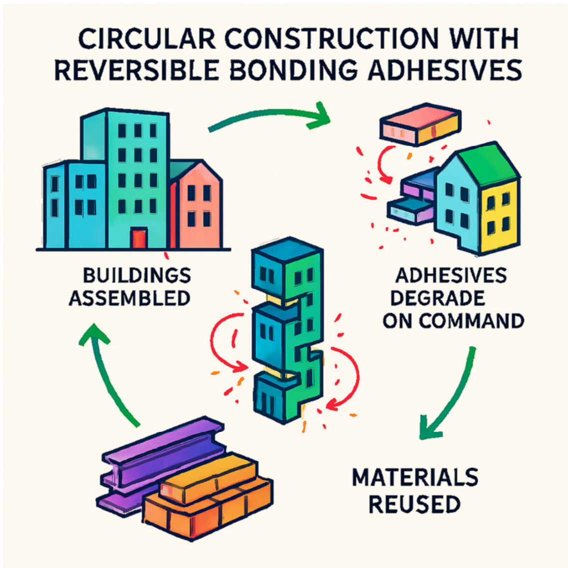


**Figure 3: Flow Chart Cycle for Green Construction Adhesive**

## VI. CONCLUSION

AI offers a powerful pathway to accelerate the design of sustainable adhesives and sealants, addressing the dual challenge of performance and sustainability. By integrating data-driven optimization with green chemistry, the construction industry can move closer to achieving low-carbon, durable, and recyclable materials. With continued advances in datasets, algorithms, and interdisciplinary collaboration, AI-optimized adhesives may soon become a cornerstone of next-generation green buildings.

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