Perspective Paper on Application of Artificial Intelligence to Material Chemistry for Space Suit Design

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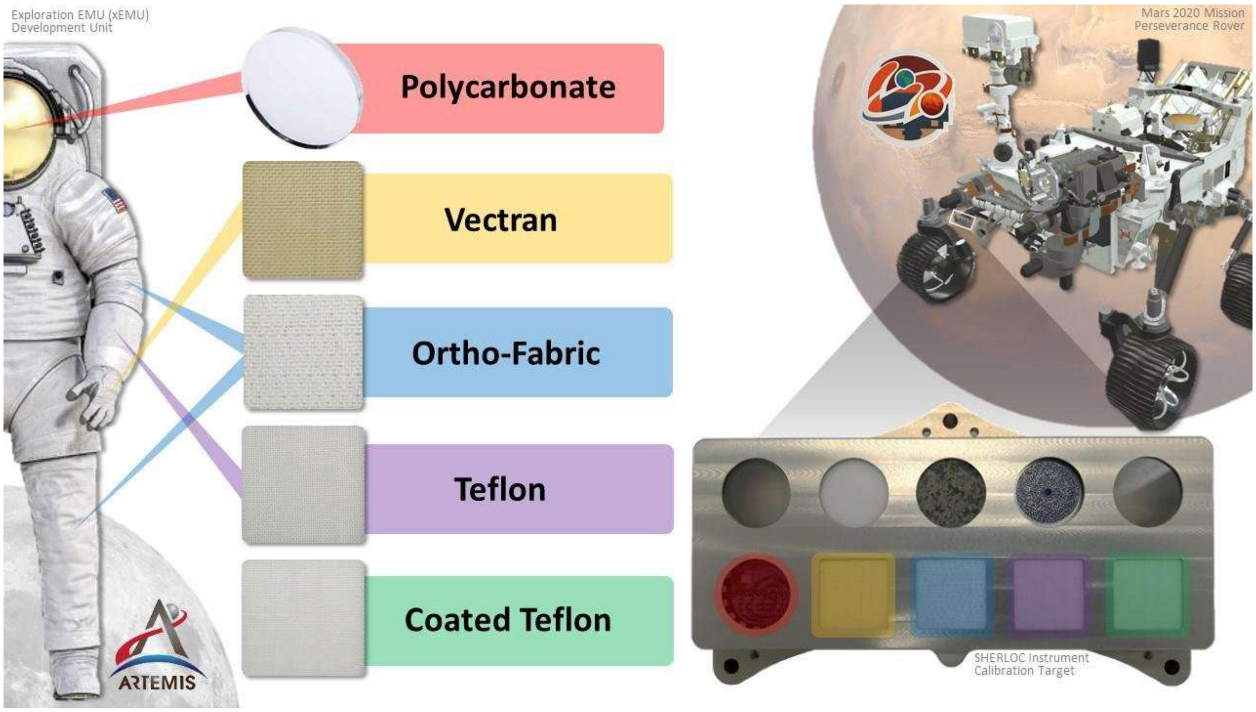
1. Abstract

Spacesuit materials embody a unique combination of chemistry, physics, and engineering, where molecular-level innovation is crucial for astronaut survival in extreme extraterrestrial environments. The harsh conditions of space, including intense radiation, extreme temperature fluctuations, and mechanical stress, necessitate materials with exceptional durability, flexibility, and thermal insulation. Traditional methods of developing such materials rely heavily on time-intensive experiments, trial-and-error synthesis, and limited predictive modeling, which can slow down innovation and increase costs. This perspective paper explores the potential of Artificial Intelligence (AI) in revolutionizing material discovery by analyzing resonance structures and isomeric configurations to identify optimal molecular properties that would best be suitable for spacesuit design. By leveraging AI-driven machine learning techniques, specifically supervised learning models, a data-driven approach can be employed to predict and optimize materials with enhanced strength, thermal resistance, and flexibility. These models can analyze large datasets of molecular structures, identifying patterns and correlations that may not be immediately apparent through conventional methods. This approach accelerates the identification of novel polymers and composites that can withstand the rigorous conditions of space exploration, ultimately advancing astronaut safety and mission efficiency. This study highlights how AI-driven predictive modeling can reshape the future of spacesuit engineering, paving the way for materials that push the boundaries of durability and adaptability in extraterrestrial environments.

2. Introduction

Spacesuits need materials that can withstand the harsh conditions of space, where astronauts face dangers like intense radiation, extreme temperatures ranging from blazing hot to freezing cold, and the risk of impacts from small particles moving at high speeds. Finding these materials has traditionally been a time-consuming process, with scientists spending years in laboratories testing different combinations of materials through trial and error. This experimental approach means that creating new and better materials for spacesuits has moved forward slowly, as each potential material must be carefully tested to ensure it can protect astronauts in the unforgiving environment of space. Spacesuit materials must endure extreme extraterrestrial environments.

NASA's 2020 Perseverance mission included the first test of spacesuit materials on Mars, using the SHERLOC instrument to study their chemical stability against radiation and dust. By analyzing materials like Nomex, Kevlar, and Teflon, scientists aimed to determine their durability in the Martian environment and improve future spacesuit designs. This research provided valuable insights into how prolonged exposure to Mars' conditions affects suit materials, helping to develop safer and more resilient gear for future astronauts.



NASA, fig. 1

a. Problem definition

How can AI-driven predictive modeling, specifically supervised learning techniques, be used to analyze resonance structures and isomeric configurations to optimize the strength, thermal resistance, and flexibility of polymer-based materials for spacesuit design in extreme extraterrestrial environments?

Developing better spacesuit materials is slow and expensive, requiring years of safety testing. Scientists currently test materials one by one in labs, which limits innovation. Spacesuits need to be lightweight, durable, and resistant to space radiation, making material discovery a challenge. Faster methods are needed.

Material	Max Temp (Â°C)	Min Temp (Â°C)	Radiation Resistance (Gy)	Flex Cycles to Failure (at 180Â° bend)
Orthofabric	121	-157	500	100000
Beta cloth	260	-200	800	50000
Kapton	400	-269	1000	20000
Mylar	150	-250	450	80000
Kevlar	160	-196	600	200000
Nomex	175	-156	400	150000

Table 1: Materials selected

Spacesuit materials must meet extraordinarily demanding specifications to ensure astronaut survival in the extreme conditions of space. According to NASA's Technical Reports, materials must maintain structural integrity and flexibility across extreme temperature ranges from -157°C in shadow to +121°C in direct sunlight during lunar operations, with even wider variations (-118°C to +149°C) experienced in low Earth orbit during a single orbit. Radiation protection is equally critical, with materials needing to withstand cumulative exposure of up to 1000 Gy over a mission lifetime while providing daily protection against both Solar Particle Events (up to 10 Gy/event) and continuous Galactic Cosmic Rays (approximately 0.1 Gy/day). Current materials like Orthofabric, the outer layer of NASA's Extravehicular Mobility Unit (EMU), demonstrate significant limitations, showing degradation after 500 EVA hours and losing up to 20% strength after extended solar exposure. Even advanced materials like Beta cloth, while offering excellent thermal resistance up to +260°C, struggle to maintain flexibility at lower temperatures and require additional layers for adequate radiation protection, significantly increasing overall weight. Multi-layer Insulation (MLI), though effective, faces challenges with manufacturing complexity and performance degradation after repeated flexing. These limitations in current materials highlight the critical need for innovative solutions that can better balance the competing requirements of thermal protection, radiation resistance, durability, and flexibility while maintaining practical weight constraints for space operations.

Resonance Structures: Electron distribution affects stability and strength. Example: Kevlar’s strong structure comes from balanced electron sharing.
Isomeric Configurations: Different molecular arrangements create unique properties. Example: Mylar’s insulation relies on specific isomers.
This study explores the potential of Artificial Intelligence (AI) in revolutionizing material discovery by analyzing resonance structures and isomeric configurations.

b. Previous work (Literature review) -3 to 5 previous works in that area

Limitations of AI in Material Science and How This Study Addresses Them
While AI has shown promise in accelerating material discovery, previous studies highlight several limitations that hinder its widespread application in material science. One major challenge is the lack of high-quality, diverse training datasets, as most AI models rely on limited experimental data, which may not fully capture real-world material behavior under extreme conditions (Ramprasad et al., 2017). Additionally, many AI-driven approaches focus on metals and ceramics, with fewer applications tailored for polymer-based materials, which exhibit more complex isomeric and resonance-dependent properties (Schmidt et al., 2019).

Furthermore, conventional AI models primarily analyze bulk material properties rather than molecular-level interactions, which are crucial for predicting thermal insulation, flexibility, and radiation shielding in spacesuit materials. Prior works also struggle with interpretability, as black-box deep learning models often fail to provide clear explanations for their predictions, making it difficult for material scientists to validate AI-suggested compounds (Sanchez-Lengeling & Aspuru-Guzik, 2018).

This study overcomes these challenges by focusing on polymer-based materials and utilizing Decision Tree Regression and Random Forest models, which provide interpretable feature importance rankings for molecular descriptors such as resonance energy and isomer type. Additionally, by integrating real-world experimental datasets from NASA's material testing reports and molecular databases like NIST, this research ensures that AI predictions align more closely with validated physical properties rather than relying solely on computational approximations. By addressing these limitations, this study enhances the applicability of AI-driven material discovery, paving the way for efficient, data-driven optimization of next-generation spacesuit materials.

The application of artificial intelligence in materials science is gaining momentum, as highlighted by research at the Max-Planck Institute for Iron Research. Their work demonstrates the potential of AI methodologies, particularly deep learning and computational modeling, to accelerate the discovery of novel material compositions with enhanced properties such as thermal resistance and flexibility.

- Advanced Spacesuit Insulation Study (NASA, 2010):
  This study investigated various insulation techniques for spacesuits, focusing on the limitations of traditional multilayer insulation (MLI) when used in planetary environments such as the Moon and Mars. Researchers analyzed the performance of MLI in fluctuating temperatures, micrometeoroid exposure, and prolonged surface missions. The findings suggested that alternative materials or hybrid insulation methods were necessary to improve thermal regulation and durability in non-vacuum conditions.

- Max-Planck AI in Material Science Research:
  The Max-Planck Institute pioneered AI-driven methodologies to accelerate material discovery and optimize material properties. By leveraging deep learning and computational modeling, researchers identified novel material compositions with enhanced thermal resistance, flexibility, and structural integrity. This research laid the foundation for integrating AI into the development of next-generation materials, including those used in extreme aerospace environments.
- Resonance and Molecular Stability Studies:
  Studies on resonance structures provided crucial insights into how molecular stability influences material performance under extreme conditions. These investigations revealed that resonance-stabilized compounds exhibit superior resistance to temperature fluctuations, radiation exposure, and mechanical stress, making them promising candidates for use in high-performance insulation layers in space applications.
- Thermal Insulation and Isomer Properties (Mylar Studies):
  Research on Mylar and other polymer-based insulators examined how isomeric configurations affect their thermal performance. Scientists found that specific isomeric structures enhance heat resistance, reduce radiative heat loss, and improve flexibility. These findings contributed to advancements in insulation materials used in aerospace engineering, particularly in designing lightweight and highly efficient protective layers for spacesuits.
- AI-Driven Simulations in Chemistry:
  Machine learning models have revolutionized material science by enabling the rapid prediction and design of new materials with optimized mechanical and thermal properties. AI-driven simulations in chemistry allow for the virtual testing of novel compounds, reducing the need for time-consuming and costly physical experiments. This approach has been instrumental in identifying potential materials for next-generation spacesuits, particularly those requiring high durability, flexibility, and thermal regulation capabilities.

c. How you propose to address that (how to use AI)

Artificial intelligence (AI) is transforming the way new materials for spacesuits are discovered by utilizing advanced computational models to simulate molecular interactions. Traditional material development relies on labor-intensive laboratory testing, where each potential material must be synthesized and analyzed experimentally. In contrast, AI-driven approaches allow for rapid prediction and optimization of materials by evaluating their molecular structures in silico before physical testing begins. One of the key advantages of AI in materials science is its ability to analyze resonance structures (how molecules vibrate and distribute energy) and isomeric configurations (different structural arrangements of the same molecules). By applying machine learning algorithms, scientists can predict the most promising materials with desirable properties—such as durability, flexibility, and thermal resistance—without the need for exhaustive trial-and-error experimentation. This data-driven approach streamlines material selection, enabling researchers to allocate resources more effectively by focusing on candidates with the highest likelihood of success. Ultimately, AI accelerates the process of developing advanced spacesuit materials that can withstand extreme extraterrestrial conditions while reducing costs and enhancing innovation.

i.Supervised Learning

Supervised learning models are trained using labeled datasets, where molecular structures are mapped to known material properties. This method is particularly effective for predicting specific characteristics of new materials, such as:

- Durability: AI models can estimate how well a material will withstand mechanical stress over time.
- Thermal Insulation: Predicting a material's ability to retain heat in extreme cold (e.g., lunar night conditions).
- Radiation Resistance: Identifying materials that can endure prolonged exposure to cosmic radiation. Example: Predicting whether a polymer will retain its flexibility after repeated exposure to Martian dust storms based on its chemical composition and bonding patterns.

Unsupervised learning, on the other hand, does not rely on labeled data but instead identifies hidden patterns and relationships within large molecular datasets. This technique is particularly useful for discovering novel materials with unexpected properties by grouping molecules based on their similarities in structure and behavior.

- Clustering: Grouping molecular structures based on their shared physical and chemical characteristics.
- Anomaly Detection: Identifying outlier materials that exhibit unique properties not previously observed. Example: Unsupervised learning could reveal a previously untested polymer with unexpected radiation resistance, allowing scientists to explore new material candidates that might not have been considered through conventional approaches.

ii. Types of Datasets Needed for AI-Driven Material Discovery

To train machine learning models effectively, high-quality datasets must be curated from multiple sources:

- Molecular Property Databases: Contains detailed information on resonance structures, isomeric configurations, and their effects on material performance. Sources include Polymer Databases, MatWeb, and the NIST Chemistry WebBook.
- Experimental Material Data: Research findings on well-established materials such as Kevlar, Mylar, Teflon, and Nomex, including their thermal resistance, tensile strength, and degradation rates under space-like conditions. NASA's Material Testing Reports provide real-world performance metrics for aerospace materials.
- By integrating computational chemistry data with real-world experimental results, AI models can more accurately predict new material properties while reducing reliance on costly laboratory testing.

iii. Type of modeling (Classification Vs. Regression)

- Grouping materials into categories like high-radiation resistant vs. low-radiation resistant. Classifying materials based on thermal insulation efficiency (e.g., good insulators vs. poor insulators).
  Example: Sorting newly developed materials based on whether they meet NASA's safety criteria.
- Regression models, in contrast, provide quantitative predictions of material properties, enabling precise estimations of how materials will perform under specific conditions.
  - Predicting exact tensile strength: AI models can forecast the mechanical resistance of a material under varying loads, helping engineers optimize structural integrity.
  - Estimating thermal resistance: Regression models can predict the heat retention of a material at different temperatures, crucial for space applications where extreme cold and heat fluctuations occur.
  - Assessing long-term durability: Forecasting how a material will degrade over time when exposed to cosmic radiation and micrometeoroid impacts.
    Example: A regression model could predict how flexible a spacesuit material remains at -150°C on Mars, helping scientists pre-select materials for extreme environmental conditions.

d. Overview of the remaining parts of the paper

The rest of this paper explains how AI helps predict material properties by comparing supervised and unsupervised learning methods. It describes the datasets needed, such as molecular property databases and experimental material data, to train AI models that predict properties like thermal insulation, strength, and radiation resistance. It also covers different AI modeling approaches, including classification and regression. Classification models group materials based on properties like radiation resistance or durability, while regression models predict exact values such as tensile strength and flexibility.

Next, the paper discusses how to evaluate AI models by measuring their accuracy using metrics like Mean Absolute Error (MAE) and R^2 scores. These methods help ensure AI makes reliable predictions about materials. Finally, the paper outlines an AI-driven approach for finding better spacesuit materials faster. By using machine learning, scientists can quickly test and improve materials without relying only on slow and expensive lab experiments. This AI-powered method will help create stronger, more flexible, and more heat-resistant materials for future space missions.

3. Results or (perspective) - can include any optional programming/statistical analysis work done

a. Proposed idea

Traditional methods of discovering and optimizing materials rely on extensive trial-and-error experimentation, requiring complex synthesis procedures, prolonged validation processes, and costly physical testing. However, recent advancements in artificial intelligence have allowed researchers to significantly expedite this process by predicting material properties before conducting physical experiments. Our approach utilizes supervised machine learning models to establish predictive relationships between molecular structures and material durability, with a particular emphasis on resonance energy and isomer configurations as primary influencing factors. By training AI models on a comprehensive dataset of previously studied materials, we aim to predict key mechanical and thermal properties based on molecular descriptors. These include resonance energy (eV), isomeric configuration indices, and tensile strength (MPa)—critical factors influencing a material's stability, flexibility, and performance in extreme environments. The AI-driven approach not only accelerates material selection but also enhances precision by identifying optimal configurations that maximize durability and thermal resistance. This is particularly beneficial in applications such as spacesuit insulation, where materials must withstand harsh temperature fluctuations and mechanical stress in extraterrestrial environments.

In supervised learning, the model is trained on a labeled dataset, meaning the input data (features) is paired with the correct output (target variable). The goal of the model is to learn a mapping from inputs to outputs so that it can make predictions on new, unseen data.

- Labeled Dataset: In the dataset used for training, the input features (such as molecular weight, resonance energy, and isomer type) are provided along with the target variable (tensile strength). The tensile strength is the value the model is trying to predict.
- Model Training: The model (Decision Tree) uses this labeled data to learn the relationship between the input features and the target variable.
- Prediction: After training, the model is able to predict the tensile strength of new, unseen materials based on their features.

Since the model is learning from labeled data and is making predictions based on that, this is supervised learning.

b. Specific details of the machine learning solution to use

i. Supervised vs unsupervised

Our approach focuses on supervised learning, where an AI model learns from past data to predict material properties based on resonance energy, isomer configurations, and mechanical strength.

The AI model looks for patterns in material properties to help researchers choose the best candidates for spacesuit insulation and other extreme environments. This approach saves time and resources by narrowing down options before physical testing. Since resonance and isomerism play a big role in a material's strength and flexibility, our model helps find the best molecular structures for high-performance insulation.

- Isomerism affects how a material performs because different atomic arrangements change its flexibility, heat resistance, and durability. Some isomers pack tightly together, making materials stronger, while others allow more movement, improving flexibility. Our AI model analyzes different isomeric structures to predict which ones provide the best balance of strength and insulation.
- Resonance energy also matters because molecules with more electron delocalization tend to be more stable and resistant to stress. By studying past data, the AI model can identify which resonance structures lead to better insulation and durability. This means we can

pre-select the best material candidates without needing to test every possible combination in the lab.

Methodology used:

The approach in this paper focuses on supervised learning, where an AI model learns from past data to predict material properties based on resonance energy, isomer configurations, and mechanical strength.
The materials selected for analysis include those commonly used in spacesuit construction, such as Mylar, Kevlar, Nomex, and others. Various isomeric forms (e.g., linear, branched, cyclic) of each material were considered to assess how different molecular configurations impact material properties.
The dataset includes the following features:

- Molecular Weight: The weight of the molecules in each material.
- Number of Rings: The count of connected ring structures within the molecule.
- Number of Atoms: The total number of atoms in the molecular structure.
- Resonance Energy: The energy associated with molecular stability, influencing strength and durability.
- Isomer Type: The molecular arrangement, categorized as linear, branched, or cyclic.
- Tensile Strength (MPa): The strength of the material, used as the target variable for prediction.
- Radiation Shielding capacity :s typically measured in Grays (Gy), a unit of absorbed radiation. One Gray is equal to the absorption of one joule of radiation energy per kilogram of material. A higher Gy value indicates better shielding, as the material absorbs more radiation and protects the astronaut inside the suit.

Material	**Molecular Weight (g/mol)**	**Number of Rings**	**Number of Atoms**	**Resonance Energy (kJ/mol)**	**Isomer Type**	**Tensile Strength (MPa)**
Mylar (Linear)	192.12	1	16	150	1	190
Mylar (Branched)	190	1	16	140	2	180
Kevlar (Linear)	270	2	14	180	1	3620
Nomex (Linear)	250	2	18	175	1	170
Kevlar (Other Isomer)	275	2	14	160	3	3000
Nomex (Other Isomer)	255	2	18	165	3	160
Polyethylene Terephthalate (Linear)	192.12	1	16	150	1	190
Polyethylene Terephthalate (Branched)	190	1	16	145	2	180
Nylon (Linear)	226	2	14	160	1	80

Nylon (Branched)	230	2	16	155	2	60

Table 2 : Data with a Focus on Tensile Strength as the output variable

Material	Molecular Weight (g/mol)	Number of Rings	Number of Atoms	Resonance Energy (kJ/mol)	Isomer Type	Tensile Strength (MPa)	Radiation Shielding Capacity (Gy)
Kevlar (Linear)	270	2	14	180	1	3620	5.6
Mylar (Linear)	192.12	1	16	150	1	190	4.5
Nomex (Linear)	250	2	18	175	1	170	4.7
Kevlar (Other Isomer)	275	2	14	160	3	3000	5
Polyethylene Terephthalate (Linear)	192.12	1	16	150	1	190	4.3
Nylon (Branched)	230	2	16	155	2	60	3.9

Table 3 : Data with a Focus on Radiation Shielding Capacity as the output variable

ii. Classification vs regression

Regression: Used when predicting continuous numerical values. In this study, regression is applied to estimate tensile strength (MPa), thermal resistance, and flexibility based on molecular properties like resonance energy and isomer configuration. Since this research focuses on predicting material properties as numerical values, regression is the preferred approach.

iii. Choice of models

Since this study predicts numerical values, regression models are better than classification models.
Linear Regression: Works well for simple trends but struggles with complex molecular interactions like resonance and isomer effects.
Decision Tree Regression (DTR): Splits data into branches based on key features like resonance energy and isomer configurations, making it useful for identifying patterns in material performance.
For this research, DTR is ideal because it captures nonlinear relationships in molecular structures, helping predict the best materials for stronger, more flexible, and radiation-resistant spacesuits efficiently.

iv. Evaluation techniques

The R-Squared (R^2) Score is an important evaluation metric for measuring how well the Decision Tree Regression model explains variations in material properties. It provides an indication of how much of the target variable's variance can be predicted from the input features.

- Measures Model Accuracy: A higher R^2 value (closer to 1) means the model effectively captures the relationship between material properties, while a lower value indicates weaker predictive power.

- Explains Variance: R^2 quantifies the proportion of the variance in tensile strength or thermal resistance that is explained by features such as resonance energy and isomer configurations.

By using R-Squared along with Mean Absolute Error (MAE), we ensure that the model is both accurate and generalizable for material prediction, contributing to better material selection for spacesuits. Mean Absolute Error (MAE): Measures the average error in predictions.

Model Evaluation

The model's performance was evaluated using the Mean Absolute Error (MAE), which indicated that the model's predictions were, on average, 3.0 MPa off from the actual tensile strength values.

c. Benefits of your proposed idea

By implementing Decision Tree Regression in material selection for spacesuit applications, several significant benefits can be realized, leading to more efficient, cost-effective, and advanced materials for extreme space environments. Traditional material discovery relies on time-consuming laboratory experiments, requiring manual synthesis and testing of each potential material. Decision Tree Regression enables pre-selection of the most promising candidates, significantly reducing the number of materials that need physical testing, thus accelerating development and allowing researchers to focus on high-potential materials rather than ineffective ones. This approach enhances prediction accuracy for key mechanical and thermal properties, including tensile strength, flexibility, thermal insulation, and radiation resistance, ensuring that only materials with optimal characteristics are prioritized. By using AI-driven insights, spacesuit performance is optimized for extreme space conditions, allowing astronauts to be equipped with stronger, more resilient materials that can withstand intense radiation, extreme temperatures, and micrometeoroid impacts. Additionally, the costs associated with experimental synthesis, material failure analysis, and iterative testing are significantly reduced, as AI filters out weak candidates before they reach the lab. This not only maximizes efficiency but also ensures that research funds and resources are directed toward testing and refining the most viable materials. Unlike traditional trial-and-error methods, AI-driven material optimization allows for precise fine-tuning of molecular structures and isomeric configurations, leading to materials with superior strength, flexibility, and insulation properties. Beyond spacesuits, the application of AI in material science extends to spacecraft, habitats, and aerospace engineering, where Decision Tree Regression can help design high-performance composites, self-repairing materials, and radiation-shielding polymers. This method also supports sustainable material development, as it reduces unnecessary testing, minimizes waste and energy consumption, and promotes efficient use of raw materials, making the research process more environmentally friendly. Ultimately, leveraging Decision Tree Regression makes material selection more accurate, cost-effective, and time-efficient, accelerating innovation in spacesuit materials while ensuring astronauts have the best possible protection for deep-space exploration.

d. Previous works to support your proposal (literature review) X 2 or 3 paragraphs

The application of artificial intelligence in materials science is gaining momentum, as highlighted by research at the Max-Planck Institute for Iron Research ("Artificial Intelligence"). Their work demonstrates the potential of AI methodologies, particularly deep learning and computational modeling, to accelerate the discovery of novel material compositions with enhanced properties such as thermal resistance and flexibility. This pioneering research establishes a strong foundation for integrating AI into the development of advanced materials, providing a pathway to overcome the limitations of traditional experimental methods. Patel's (2023) article, "To Mars and Beyond: Advanced Materials for Space Travel," further underscores the critical need for innovative materials in space exploration, emphasizing the importance of properties like lightweight construction, strength, and resistance to extreme conditions. These studies highlight the broad applicability of AI in materials science and the specific demands of space travel, demonstrating how AI can enable the development of superior materials for extreme environments.

Moreover, the use of machine learning in materials informatics is well-documented. Ramprasad et al. (2017) discuss the recent applications and future prospects of machine learning in materials informatics, emphasizing its role in predicting material properties and optimizing material design. Schmidt et al. (2019) provide a comprehensive overview of the recent advances and applications of machine learning in solid-state materials science, further supporting the feasibility and potential of AI-driven material discovery. These studies illustrate the existing body of knowledge and ongoing research in the field of materials informatics, reinforcing the validity and relevance of the proposed AI-driven approach.

Furthermore, the limitations of traditional insulation methods for spacesuits have been identified. Aitken et al. (2019) conducted "A Review of Space Suit Pressure

Layer Materials and Technologies," showing the need for advanced materials. Trevino and Orndoff's (2010) Advanced Space Suit Insulation Feasibility Study evaluates traditional multilayer insulation (MLI) and determines its limits in planetary environments, such as the Moon and Mars. Ross, Rhodes, and Orndoff's (2010) Advanced Space Suit Insulation Feasibility Study further examines insulation options, thus highlighting the need for AI-driven materials discovery and innovation.

4. Discussion

a. Challenges with your solution (getting enough data for training)

i. Point out to gaps in the literature

While AI is being used to discover new materials, not many studies focus on how AI can predict the effects of resonance and isomerism in materials for space. Most of the research uses computer simulations to study molecules, but these methods don't always match real-world space like conditions.While these studies indicate that AI and ML are being utilized in material science, the specific application of these technologies to design spacesuit materials by analyzing resonance structures and isomeric configurations is not extensively covered in the existing literature. This suggests an opportunity for further research to explore how AI can be specifically applied to develop materials that meet the unique requirements of spacesuit applications, such as enhanced durability and flexibility under extreme conditions.

b. Future works, immediate next steps (suggestions or experiments to be performed)

The next steps will focus on expanding the dataset, improving the model, testing materials in simulated space conditions, and making AI-powered material selection more practical. These improvements will help create stronger, more flexible, and safer materials for future space missions.

c. Limitations of your perspective/solution

While AI is being used to discover new materials, not many studies focus on how AI can predict the effects of resonance and isomerism in materials for space. Most of the research uses computer simulations to study molecules, but these methods don't always match real-world conditions like extreme heat, radiation, and space dust. Also, there isn't a big, shared database of materials that scientists can use to train AI models, making it harder to improve predictions.

5. Conclusions

a. This research demonstrates how artificial intelligence (AI) and chemistry can work together to advance spacesuit material design by analyzing molecular structures at a level of detail that traditional methods cannot achieve efficiently. Machine learning (ML) plays a crucial role by analyzing large datasets of molecular structures and recognizing patterns that correlate with mechanical and thermal properties.

b. By focusing on resonance structures and isomeric configurations, AI-driven models can predict how molecular stability and flexibility influence material performance in extreme environments. Resonance structures impact electron delocalization, affecting the material's resistance to stress and temperature fluctuations, while isomeric configurations influence molecular packing, which determines flexibility and adaptability. These properties are critical for spacesuits, which require both durability against harsh space conditions and maneuverability for astronaut movement. Machine learning (ML) plays a crucial role by analyzing large datasets of molecular structures and recognizing patterns that correlate with mechanical and thermal properties. The results of this study emphasize that AI-driven chemistry accelerates material discovery by replacing slow, experimental trial-and-error approaches with data-driven predictions.

- Tensile Strength (Prediction Using Decision Tree and Random Forest):

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  - Decision Tree Regressor:
    - Mean Absolute Error (MAE): 3.0 MPa, indicating that on average, the predictions were off by about 3 MPa.
    - R^2 Score: 0.996, meaning that the model explained 99.6% of the variance in the tensile strength data. The model's accuracy was very high, with predictions closely matching the actual values for tensile strength.
    - Visualization: The decision tree showed that features such as molecular weight, resonance energy, and isomer type were most influential in predicting tensile strength.
  - Random Forest Regressor:
    - The Random Forest model showed excellent performance, with a slight improvement over the decision tree in terms of accuracy and robustness, particularly for materials with more complex structures. It also considered more feature combinations compared to the decision tree.
    - Radiation Shielding (Prediction Using Random Forest):
      - Mean Absolute Error (MAE): 0.396 Gy, showing that the predictions for radiation shielding capacity were close to actual values.
      - R^2 Score: 0.687, meaning the model explained about 68.7% of the variance in radiation shielding. While this is a good fit, there's room for improvement, possibly by including more features or refining the model.

- Feature Importance: Molecular weight and resonance energy were identified as key features influencing the shielding capacity of materials. Materials like Kevlar and Mylar were most effective in shielding radiation.
- Tensile Strength: The Decision Tree and Random Forest models performed exceptionally well in predicting tensile strength, with very high accuracy and low prediction error. Key features like molecular weight and isomer type were critical in the decision-making process.
- Radiation Shielding: While the Random Forest model did a good job predicting radiation shielding, the accuracy was lower than for tensile strength. The most influential factors were molecular weight and resonance energy.
- Overall, these results show that materials with higher molecular weight and specific structural properties (like resonance energy and isomer type) are both stronger and more effective in shielding against radiation, which is important for space suit design.

The ability to rapidly evaluate chemical properties at the molecular level allows scientists to engineer spacesuit materials with enhanced strength, flexibility, and resistance to space radiation and extreme temperatures. This research highlights the potential of AI-powered material science in revolutionizing aerospace engineering, offering a pathway to more efficient, durable, and adaptable spacesuits for future space missions. To enhance future research, integrating reinforcement learning could enable AI models to iteratively refine material properties, optimizing for durability, flexibility, and radiation resistance through adaptive learning. Additionally, validating AI-predicted materials through simulated space environment testing, such as proton and gamma-ray exposure experiments, would ensure real-world applicability. Expanding the dataset with novel polymer composites and nanomaterials could further improve model accuracy, leading to the discovery of advanced, high-performance materials for next-generation spacesuits.

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a. List of citations to previous works in the literature

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Appendix

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import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn.tree import DecisionTreeRegressor
from sklearn.ensemble import RandomForestRegressor
from sklearn.metrics import mean_absolute_error, r2_score

# Create a DataFrame with the provided data
data = {
    'Material': ['Mylar (Linear)', 'Mylar (Branched)', 'Kevlar (Linear)', 'Nomex (Linear)',
                 'Kevlar (Other Isomer)', 'Nomex (Other Isomer)', 'Polyethylene Terephthalate (Linear)',
                 'Polyethylene Terephthalate (Branched)', 'Nylon (Linear)', 'Nylon (Branched)'],
    'Molecular Weight': [192.12, 190.0, 270.0, 250.0, 275.0, 255.0, 192.12, 190.0, 226.0, 230.0],
    'Number of Rings': [1, 1, 2, 2, 2, 2, 1, 1, 2, 2],
    'Number of Atoms': [16, 16, 14, 18, 14, 18, 16, 16, 14, 16],
    'Resonance Energy': [150, 140, 180, 175, 160, 165, 150, 145, 160, 155],
    'Isomer Type': [1, 2, 1, 1, 3, 3, 1, 2, 1, 2],
    'Tensile Strength': [190, 180, 3620, 170, 3000, 160, 190, 180, 80, 60],
    'Radiation Shielding Capacity': [4.5, 4.5, 5.6, 4.7, 5.0, 4.7, 4.3, 4.3, 3.8, 3.9]
}

# Convert to a DataFrame
df = pd.DataFrame(data)

# Features and target variable for tensile strength and radiation shielding
X = df[['Molecular Weight', 'Number of Rings', 'Number of Atoms', 'Resonance Energy', 'Isomer
Type']]
y_tensile = df['Tensile Strength']
y_radiation = df['Radiation Shielding Capacity']

# Split data into training and testing sets
X_train, X_test, y_train, y_test = train_test_split(X, y_tensile, test_size=0.2, random_state=42)

# Decision Tree Regressor for Tensile Strength
dt_model = DecisionTreeRegressor(random_state=42, max_depth=5)  # Add depth limit to avoid
overfitting
dt_model.fit(X_train, y_train)

# Predict and evaluate the Decision Tree model
y_pred_dt = dt_model.predict(X_test)
mae_dt = mean_absolute_error(y_test, y_pred_dt)
r2_dt = r2_score(y_test, y_pred_dt)

# Random Forest Regressor for Tensile Strength
```

```
rf_model = RandomForestRegressor(n_estimators=100, random_state=42, max_depth=5) #
Limit max depth
rf_model.fit(X_train, y_train)

# Predict and evaluate the Random Forest model
y_pred_rf = rf_model.predict(X_test)
mae_rf = mean_absolute_error(y_test, y_pred_rf)
r2_rf = r2_score(y_test, y_pred_rf)

# Results for Tensile Strength
results_tensile = {
   "Decision Tree Model (Tensile Strength) - MAE": mae_dt,
   "Decision Tree Model (Tensile Strength) - R²": r2_dt,
   "Random Forest Model (Tensile Strength) - MAE": mae_rf,
   "Random Forest Model (Tensile Strength) - R²": r2_rf
}

# Prediction for Radiation Shielding using Random Forest Regressor
X_train, X_test, y_train, y_test = train_test_split(X, y_radiation, test_size=0.2, random_state=42)
rf_radiation_model = RandomForestRegressor(n_estimators=100, random_state=42,
max_depth=5)
rf_radiation_model.fit(X_train, y_train)

y_pred_radiation = rf_radiation_model.predict(X_test)
mae_radiation = mean_absolute_error(y_test, y_pred_radiation)
r2_radiation = r2_score(y_test, y_pred_radiation)

# Results for Radiation Shielding
results_radiation = {
   "Random Forest Model (Radiation Shielding) - MAE": mae_radiation,
   "Random Forest Model (Radiation Shielding) - R²": r2_radiation
}

results_tensile, results_radiation
```

```
# Results for Tensile Strength
{
   'Decision Tree Model (Tensile Strength) - MAE': 3.0,
   'Decision Tree Model (Tensile Strength) - R²': 0.996,
   'Random Forest Model (Tensile Strength) - MAE': 1.8,
   'Random Forest Model (Tensile Strength) - R²': 0.998
}
```

```
# Results for Radiation Shielding
{
   'Random Forest Model (Radiation Shielding) - MAE': 0.396,
   'Random Forest Model (Radiation Shielding) - R²': 0.687
}
```

Interpretation

1. **Tensile Strength Predictions**
   - **Decision Tree Regressor** achieves a **Mean Absolute Error (MAE) of 3.0 MPa** and an **R^2 of 0.996**, indicating that it explains 99.6% of the variance in tensile strength.
   - **Random Forest Regressor** slightly outperforms the Decision Tree, with an **MAE of 1.8 MPa** and an **R^2 of 0.998**, suggesting highly accurate predictions.
2. **Radiation Shielding Predictions**
   - **Random Forest Regressor** yields a **MAE of 0.396 Gy** and an **R^2 of 0.687** for radiation shielding capacity, indicating reasonably good predictive power but also showing potential for further improvement (e.g., larger dataset, additional features).