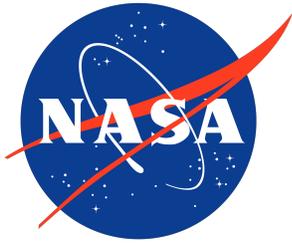


NASA/TM-20250009373



An Overview on Designable Adhesion for Aviation Applications

*A. Mark Settles and John W. Lawson
Ames Research Center, Moffett Field, CA*

*Christopher E. Porter
Glenn Research Center, Cleveland, OH*

*Cheol Park, Michael D. Patterson, and Brandon E. Sells
Langley Research Center, Hampton, Virginia*

*Christopher Giuffre
HX5 LLC, Glenn Research Center, Cleveland, OH*

*Emmanouil T. Skountzos, Andrew P. Latham, and Ashwin Ravishandran
KBR Inc., Ames Research Center, Moffett Field, CA*

NASA STI Program Report Series

Since its founding, NASA has been dedicated to the advancement of aeronautics and space science. The NASA scientific and technical information (STI) program plays a key part in helping NASA maintain this important role.

The NASA STI Program operates under the auspices of the Agency Chief Information Officer. It collects, organizes, provides for archiving, and disseminates NASA's STI. The NASA STI Program provides access to the NTRS Registered and its public interface, the NASA Technical Report Server, thus providing one of the largest collections of aeronautical and space science STI in the world. Results are published in both non-NASA channels and by NASA in the NASA STI Report Series, which includes the following report types:

- **TECHNICAL PUBLICATION.** Reports of completed research or a major significant phase of research that present the results of NASA programs and include extensive data or theoretical analysis. Includes compilations of significant scientific and technical data and information deemed to be of continuing reference value. NASA counterpart of peer-reviewed formal professional papers, but having less stringent limitations on manuscript length and extent of graphic presentations.
- **TECHNICAL MEMORANDUM.** Scientific and technical findings that are preliminary or of specialized interest, e.g., quick release reports, working papers, and bibliographies that contain minimal annotation. Does not contain extensive analysis.
- **CONTRACTOR REPORT.** Scientific and technical findings by NASA-sponsored contractors and grantees.

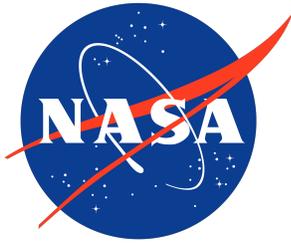
- **CONFERENCE PUBLICATION.** Collected papers from scientific and technical conferences, symposia, seminars, or other meetings sponsored or co-sponsored by NASA.
- **SPECIAL PUBLICATION.** Scientific, technical, or historical information from NASA programs, projects, and missions, often concerned with subjects having substantial public interest.
- **TECHNICAL TRANSLATION.** English-language translations of foreign scientific and technical material pertinent to NASA's mission.

Specialized services also include organizing and publishing research results, distributing specialized research announcements and feeds, providing information desk and personal search support, and enabling data exchange services.

For more information about the NASA STI Program, see the following:

- Access the NASA STI program home page at <http://www.sti.nasa.gov>
- Help desk contact information: <https://www.sti.nasa.gov/sti-contact-form/> and select the "General" help request type.

NASA/TM-20250009373



An Overview on Designable Adhesion for Aviation Applications

*A. Mark Settles and John W. Lawson
Ames Research Center, Moffett Field, CA*

*Christopher E. Porter
Glenn Research Center, Cleveland, OH*

*Cheol Park, Michael D. Patterson, and Brandon E. Sells
Langley Research Center, Hampton, Virginia*

*Christopher Giuffre
HX5 LLC, Glenn Research Center, Cleveland, OH*

*Emmanouil T. Skountzos, Andrew P. Latham, and Ashwin Ravishandran
KBR Inc., Ames Research Center, Moffett Field, CA*

National Aeronautics and
Space Administration

Ames Research Center
Moffett Field, CA 94035

September 2025

Acknowledgments

This work was funded by NASA's Convergent Aeronautics Solutions (CAS) project in the Transformative Aeronautics Concepts Program (TACP) of the Aeronautics Research Mission Directorate (ARMD).

The use of trademarks or names of manufacturers in this report is for accurate reporting and does not constitute an official endorsement, either expressed or implied, of such products or manufacturers by the National Aeronautics and Space Administration.

Abstract

Novel adhesive materials have the potential to enable step changes in transformational aircraft both in the manufacture, operations, and maintenance phases of a vehicle's life cycle. A variety of barriers, both technological and regulatory, stand in the way of adopting novel adhesive technologies. This paper provides a system level analysis on the impact of adhesive technologies on the Advanced Air Mobility market. Additionally, an overview of state-of-the-art capabilities are discussed for three distinct areas of adhesion: 1) low ice adhesion coatings, 2) strong adhesives for structural bonding, and 3) bio-engineered adhesive technologies. This effort identified the need for more tightly coupling computational and experimental research activities to accelerate adhesive material design.

Contents

1	Introduction	6
2	A Motivating Need for Adhesive Technologies in Advanced Air Mobility	6
2.1	Introduction to AAM and Potential Benefits of Designed Adhesive Technologies	7
2.2	AAM Business Viability for Low-ice Adhesion	8
2.2.1	Icing Impacts on Potential Operations	9
2.2.2	Icing Impacts on Operation Economics	11
2.3	AAM Business Viability for Structural Adhesion	13
2.4	Summary of Potential Benefits to AAM	17
3	Low Ice Adhesion Material Design and Evaluation	18
3.1	Computational Design	18
3.2	Experimental Evaluation	21
3.2.1	Background	21
3.2.2	Ice Adhesion Testing at NASA	23
4	Structural Bonding	24
5	Bio-engineered Adhesives	26
5.1	Bioengineered Polymer Design	26
5.2	Role of Modeling and Simulation in Designing Bio-inspired Coating Materials for Aeronautics Applications	28
5.3	Potential for Biohybrid Coatings and Adhesives	30
6	Discussion	31

Nomenclature

<i>AAM</i>	Advanced Air Mobility
<i>ARMD</i>	Aeronautics Research Mission Directorate
<i>BN</i>	Boron Nitride
<i>CEF</i>	Cost Escalation Factor
<i>DOC</i>	Direct Operating Cost
<i>eVTOL</i>	Electric Vertical Takeoff and Landing
<i>FIKI</i>	Flight into Known Icing
<i>NASA</i>	National Aeronautics and Space Administration
<i>MD</i>	Molecular Dynamics
<i>RAM</i>	Regional Air Mobility
<i>TRL</i>	Technology Readiness Level
<i>QLL</i>	Quasi-Liquid Layer
<i>UAM</i>	Urban Air Mobility

List of Figures

1	Percentages of simulated Regional Air Mobility flights completed (orange) and cancelled due to icing (maroon) across the Northeast corridor and greater Colorado region. Adapted from Ref. [1].	9
2	Percentages of simulated Urban Air Mobility flights impacts due to icing-related weather (maroon) and otherwise (orange) for the Chicago and Dallas metro areas. Icing-related weather is characterized as either low temperature, snow, freezing rain, freezing drizzle, snow grains, snow crystals, or combinations thereof. Adapted from Ref. [2].	10
3	Estimated number of daily operations enabled for the Chicago, Dallas, New York City, and Denver metro areas. The estimations are based on knock-down factors observed in Figs. 1 and 2 and represent the scale of flights that aircraft equipped with a notional anti-icing adhesive technology could perform.	11
4	Lift-Plus-Cruise Urban Air Mobility Reference Vehicle. [3]	12
5	Percentages of estimated direct operating cost savings for notional 25 and 50 nautical mile average trips. The percentages represent the threshold of savings available with anti-icing materials that are capable of enabling 20% of flights that would otherwise have been canceled due to icing conditions.	13
6	Estimated cost breakdown and comparison of a baseline eVTOL aircraft and a notional eVTOL aircraft integrated with designed adhesion technology using an adapted version of the modified DAPCA-IV cost estimating relationship model [4] [5].	15
7	Unit selling price estimates as a function of the units produced over time for a baseline eVTOL aircraft and a notional eVTOL aircraft integrated with designed adhesion technology. The figure includes data callouts for the baseline (upper) and eVTOL aircraft integrated with designed adhesion technology (lower) for reference. The production rates for the notional eVTOL with designed adhesion technology are modeled up to 2000 units produced over five years to estimate the cost impact of increased production rates over the baseline due to the adhesion technology.	16
8	Estimated gross profits of the baseline eVTOL and the eVTOL integrated with designed adhesion technology with an estimated “breakeven” point superposed in black at approximately 60M USD at 1,045 units. The 1,045 units translate to nine additional aircraft per year over five years. The eVTOL aircraft with designed adhesion technology is estimated to outpace the gross profit of the baseline eVTOL aircraft if the technology enables higher production rates.	17
9	Representative atomic configurations of: (a) graphite/ice, (b) BN/ice and (c) epoxy/ice systems, as obtained from MD simulations. Reprinted with permission from Ref. [6]. Copyright 2024 American Chemical Society.	20

10	Modified lap joint shear samples in the IRT (left) and experimental lap shear apparatus (right).	23
11	Process for automatically determining grain boundaries via machine learning.	24
12	MD simulation evidence of growth of an ice nuclei into a 3D ice nanocrystal on the ice binding surface of TmAFP. The central backbone of the protein is depicted using a silver cartoon representation, while the functional groups on the ice binding surface are highlighted with sticks (C - blue; O - red; H - white). The water molecules in the liquid are represented by red spheres, whereas those in the ice-like layers are represented by blue-white spheres. Image modified from ref. [89] CC BY 4.0.	29

1 Introduction

High and low adhesive materials are desirable from an engineering perspective due to the potential ease for integration within the manufacture and operations of flight vehicles. For instance, imagine a paint or coating that could be applied to the surface of a wing, rotor, or engine fan that would keep that component free of ice. This would effectively eliminate the need for conventional thermal, boot, or glycol based anti-icing systems that have non-negligible size weight and power requirements. Or imagine a structural adhesive that could bond two complex mating surfaces together with the reliability and strength of conventional mechanical fasteners, reducing weight and increasing vehicle production.

While these solutions are attractive from a conceptual stand point, practically speaking the technology is still at too low of a Technology Readiness Level (TRL) to completely replace conventional anti-icing systems or mechanical fasteners. One of the challenges that stands in the way is the design and development of novel materials. Existing substrates and adhesives are primarily used in industry and actively researched. However, the development of new, tailored substrates and adhesives is difficult and challenging due to the cost around fabrication and evaluation. Recently computational efforts have shown promise in understanding the physical phenomenon associated with adhesion. This physical understanding shows the potential to allow a coupled computational/experimental practice to design tailored adhesive solutions for their particular applications.

Additionally, the adhesive properties of a material is just one of many design aspects that are of importance for adoption in aviation. Other considerations such as installation repeatability, physical durability, ultra violet resistance, and fatigue are just a few additional properties of interest for low ice adhesion substrates and structural adhesives. To that end, it seems natural to develop an extensible design method to allow for the inclusion of additional design parameters of interest. Thus, while the focus of this effort is to identify how to design materials for their adhesive properties, the tools and methods should allow for extension to incorporate other design parameters that may be of interest in the future.

This paper details the pre-execution activities of the Designed Adhesion effort in NASA's Convergent Aeronautic Solutions (CAS) project. Specifically a system analysis study of the potential impacts of designable adhesion for advanced air mobility (AAM) market. Additionally, summaries of the state-of-the-art in three distinct areas of adhesion are detailed. These three areas are: 1) low ice adhesion coatings, 2) strong adhesives for structural bonding, and 3) bio-engineered adhesive technologies.

2 A Motivating Need for Adhesive Technologies in Advanced Air Mobility

Although the materials and research discussed in this paper may be applied to many domains, we will motivate our work by focusing on one particular area of application: advanced air mobility. In this section we provide an introduction to

AAM along with background research and simple analyses that motivate exploring new adhesion technologies to benefit AAM aircraft and operations.

2.1 Introduction to AAM and Potential Benefits of Designed Adhesive Technologies

There is growing interest in the field of advanced air mobility (AAM), which envisions novel, small aircraft performing relatively short-range missions that provide aviation services to more places for more people to utilize. There is no universally agreed upon definition of AAM, but one is safe, sustainable, affordable, and accessible aviation for transformational local and intraregional missions [7]. These transformational missions are believed to be enabled by a convergence of new aviation technologies, such as electrified aircraft propulsion and increased levels of automation in aircraft and air traffic management, and emerging business models, such as mobile application-based ridesharing. AAM is typically described as having at least two major components: urban air mobility (UAM) and regional air mobility (RAM). UAM [8] [9] is generally focused on local transportation around metropolitan areas, which implies trips are generally less than about 50 miles. Many envision UAM specifically as passenger transport missions in novel electric vertical takeoff and landing (eVTOL) aircraft flying among a network of takeoff and landing areas called vertiports [10]. RAM [11] involves “intraregional” missions, between approximately 50 and 500 miles in range, that are often envisioned to leverage existing airport infrastructure and conventional or short takeoff and landing aircraft. Passenger-carrying aircraft for both UAM and RAM are generally envisioned to be between one and thirty passengers, with many in the five to nine passenger range.

There are many challenges that must be overcome before AAM can become ubiquitous, including reducing costs and noise compared to existing aviation, developing additional infrastructure from which aircraft can takeoff and land, enabling flight in many different weather conditions, and safely managing air traffic [12] [13]. The novel adhesive materials discussed in this paper may help overcome some, but certainly not nearly all, of these challenges.

To reach the levels of scale proposed by entities like Uber Elevate [9], advancements in manufacturing that reduce manufacturing costs and can be scaled to large production volumes are required. Adhesives represent one means through which these cost reductions and production volume increases may be achieved, since automated processes can be leveraged to apply the adhesives in production. Additionally, adhesives may lead to lower aircraft weights and reduce inspection times from reduced fastener counts, which can also help reduce costs [14].

For AAM to be a reliable, year-round transportation option and reap the cost benefits of high aircraft utilization, aircraft must demonstrate the ability to operate in a wide variety of weather conditions, including potential icing conditions. Low-ice adhesion materials may provide means for AAM aircraft, which are generally envisioned to be constrained in both weight and energy, to pragmatically operate in more weather conditions than typical general aviation aircraft, without the weight and power requirements of traditional anti-icing systems [14]. Furthermore, even if flight into known icing (FIKI) certification cannot ultimately be achieved with

low-ice adhesion materials, these materials may enable AAM aircraft to maintain operational flexibility when there is inadvertent flight into icing conditions. Specifically for powered-lift ¹ aircraft, which includes many eVTOL aircraft, that transition from wingborne flight in cruise to thrustborne flight for vertical landings, inadvertent icing encounters could lead to thrust reductions that may preclude them from transitioning from wingborne to thrustborne flight. In such an event, the aircraft would likely have to divert to land on a conventional runway in fixed-wing mode instead of landing vertically at a vertiport, which could increase required energy reserves ² for UAM operations when icing conditions could be present. Because eVTOL aircraft are generally energy constrained, these increased operational energy reserve requirements could significantly constrain the routes these aircraft can fly on days with icing potential, limiting their usefulness and revenue-generating potential. Low-ice adhesion materials offer the potential for powered-lift aircraft to still inadvertently encounter icing conditions for a short period of time without the performance degradations that would necessitate a conventional landing by enabling the aerodynamic surfaces to avoid any ice accretion. Thus, these low-ice adhesion materials may enable greater economic productivity from the aircraft by enabling the same routes to be flown on days without known icing but with icing potential.

In the following subsections, we build on previous work [15] [16] [2] [17] [18] [19] [20] and describe some simple analyses to roughly quantify the impact of low-ice adhesion and structural adhesion. The insights from the analysis documented in this paper address the potential operational and economic impacts of icing on AAM operations and the potential economic impact of large-scale production using structural adhesion. The operational and economic impacts for both the low-ice adhesion and structural adhesion elements provide insight into the business viability of would-be designed-adhesive technologies for AAM.

2.2 AAM Business Viability for Low-ice Adhesion

Across the Advanced Air Mobility community, efforts from industry leaders, government entities, and academia collectively bring AAM closer to initial operations. Some stakeholders consider AAM operations to include year-round operations, and thus require anti-ice technologies to sustain cold-weather operations for both passenger-carrying and cargo missions. Low-ice adhesion technologies may be an innovation that helps reduce aircraft downtime by extending operational capabilities in adverse weather conditions, reducing delays in cargo deliveries and improving reliability for passenger flights.

To inform AAM business viability, we analyzed the expected number of flights impacted by icing and icing related weather, the expected number of enabled operations with a notional anti-icing technology, and the expected direct operating

¹A powered-lift aircraft is "a heavier-than-air aircraft capable of vertical takeoff, vertical landing, and low speed flight that depends principally on engine-driven lift devices or engine thrust for lift during these flight regimes and on nonrotating airfoil(s) for lift during horizontal flight". (14 CFR 1.1)

²In the Federal Aviation Regulations (i.e., Title 14 of the Code of Federal Regulations), energy reserves are termed "fuel" reserves. We use energy here because all-electric aircraft have no traditional fuel.

cost savings available if FIKI is enabled. The analysis leverages previous research efforts to understand the expected demand and market for both Regional Air Mobility [18] [19] [20] [1] and Urban Air Mobility [15] [16] [2] [17] in particular areas of the U.S. These RAM and UAM studies use historical travel demand from the U.S. Census supplemented with flights from existing operators, as available, to model representative Federal Aviation Regulations Part 135 operations with notional aircraft. The RAM studies analyzed the Northeast Corridor and the Greater Colorado Region, and the UAM studies examined operations across the Chicago, Dallas, New York City, and Denver metro areas. Additional details and study assumptions are listed in the respective references.

2.2.1 Icing Impacts on Potential Operations

We first sought to understand the potential number of operations that may be impacted by icing across the regional and urban air mobility missions to inform the business viability of a low-ice adhesive technology. For the RAM use case, given notional demand and historical weather information from 2017-2018, Kim et al. found that roughly 20% of the simulated Part 135 flights would be cancelled solely due to icing in the Northeast corridor and greater Colorado regions [1]. Figure 1 illustrates the percent of notional RAM flights that could be completed (orange) or would have to cancel due to icing (maroon). Despite the differences in the route structure and weather patterns across both locations, both the Northeast corridor and the greater Colorado area exhibited similar estimated outcomes. Because of this similarity in the net result of canceled operations across different regions, we assume that this 20% cancellation factor, applied to the number of potential operations, may be applicable across similar regions with predominately cold climates in some of our following analysis.

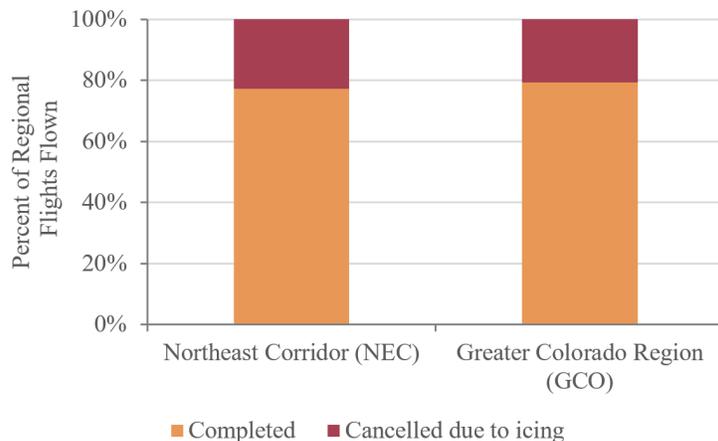


Figure 1. Percentages of simulated Regional Air Mobility flights completed (orange) and cancelled due to icing (maroon) across the Northeast corridor and greater Colorado region. Adapted from Ref. [1].

For the UAM use case, demand was modeled for notional flights leveraging data

on existing trips taken on the ground; a portion of those existing trips were modeled to select the UAM mode as being a preferred means of travel based on the effective cost (also known as the generalized cost) of the trip [16]. Chao et al. analyzed the potential impacts of weather on these predicted UAM trips based on methods from Goyal et al. [21] by studying historical weather information as reported by weather stations located on the ground from 2019 in the Chicago and Dallas areas [2]. Leveraging the analysis from Chao et al., we extracted instances of weather that would potentially lead to icing conditions to ascertain what percentage of UAM trips may be affected by icing-related weather. Icing-related weather is characterized as either low temperature, snow, freezing rain, freezing drizzle, snow pellets, snow grains, and ice crystals or combinations thereof ³. Figure 2 illustrates the percentages of notional urban flights that would have been impacted by icing-related weather (maroon) and those unaffected by icing-related weather (orange) based on 2019 weather data. This analysis indicates that there is an order-of-magnitude difference in the number of simulated flights impacted due to icing-related weather between Chicago (16%), which has a predominately cold climate, and Dallas (1.6%), which has a humid sub-tropical climate. Although the weather analysis of Chao et al. estimated weather impacts specifically for Chicago and Dallas, we assume that the rough-order-of-magnitudes of flights potentially impacted by icing conditions for those two areas can be extended to areas with similar climates to estimate the number of impacted operations in future analyses.

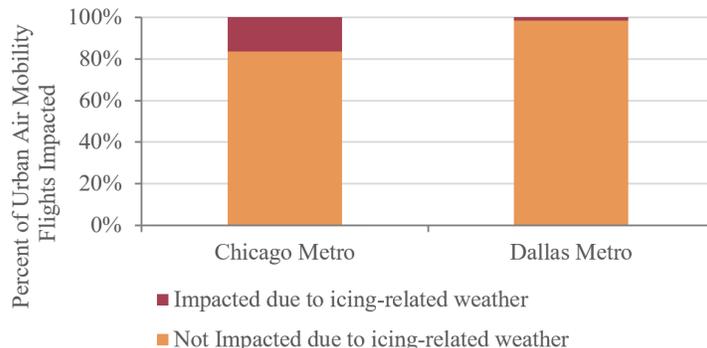


Figure 2. Percentages of simulated Urban Air Mobility flights impacts due to icing-related weather (maroon) and otherwise (orange) for the Chicago and Dallas metro areas. Icing-related weather is characterized as either low temperature, snow, freezing rain, freezing drizzle, snow grains, snow crystals, or combinations thereof. Adapted from Ref. [2].

The total number of daily operations enabled by a notional anti-icing technology was estimated with a 20% cancellation rate from Fig. 1 applied to the New York City and Denver UAM trip data from Ref. [17], the 16% rate of icing-impacted

³Since the data from Chao et al. only considered ground-based weather reporting stations, the analysis may underpredict instances of icing-related weather at altitude. However, since UAM aircraft are generally envisioned to fly at low altitudes of up to a few thousand feet, the effects of altitude are not as large as in traditional aviation.

flights from Fig. 2 applied to the Chicago UAM trip data from Ref. [17], and the 1.6% rate of icing-impacted flights from Fig. 2 applied to the Dallas UAM trip data from Ref. [17]. Although the 20% rate of flight cancellations due to icing from Kim et al. represent RAM missions, the team leveraged this rate for UAM as an initial estimate; we acknowledge that this may be higher than would be experienced in practice for lower-altitude UAM missions. Edsel et al. estimate the total number of daily flights in Chicago, Dallas, New York, and Denver to be 6,240, 188, 21,107, and 4,490, respectively. Across the metro areas, the estimated number of operations that experience icing or icing-related weather and could be flown with an anti-icing capability scales from hundreds for the Dallas metro to tens of thousands in the New York City metro, shown in Fig. 3. The predicted impact for Dallas is considered marginal with the number of enabled trips on the order of 10^2 (188). Metro areas like Chicago and Denver are considered moderately impacted with an order of 10^3 with 6,240 and 4,490 enabled operations, respectively. The New York City metro area eclipsed all other areas with a large, predicted impact on the order of 10^4 with 21,107 enabled operations. Since the expected demand for operations in the New York City area far exceeds what is predicted for Chicago and Denver, the estimated number of enabled operations is three to four times greater.

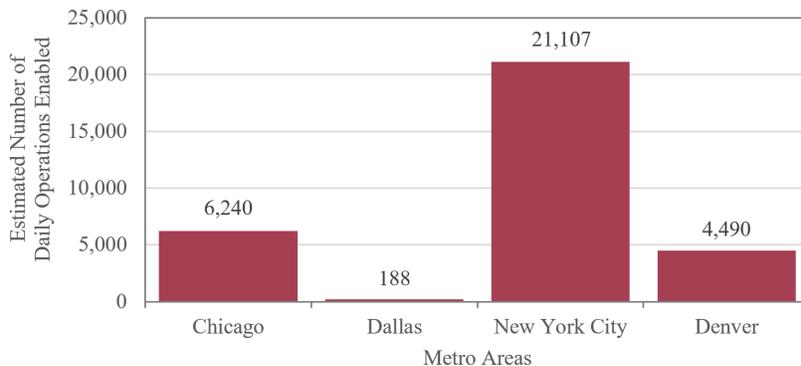


Figure 3. Estimated number of daily operations enabled for the Chicago, Dallas, New York City, and Denver metro areas. The estimations are based on knock-down factors observed in Figs. 1 and 2 and represent the scale of flights that aircraft equipped with a notional anti-icing adhesive technology could perform.

2.2.2 Icing Impacts on Operation Economics

The economics of operating eVTOL aircraft for UAM is based on several factors related to aircraft characteristics, concept of operations, infrastructure, energy, and the frequency of operations. The systems analysis leveraged a direct operating cost (DOC) model from Refs. [22] [23] to estimate the cost per flight hour and operating cost per passenger based on the maximum gross takeoff weight, passenger capacity, battery energy capacity, expected trip distances, and average block speed. The analysis modeled the fully electric variant of the NASA Lift-Plus-Cruise (also written as lift+cruise) UAM reference aircraft [3] [24] due to its modeling maturity

and documentation. The lift+cruise reference vehicle has a fixed wing configuration with eight lifting rotors and one pusher propeller, as shown in Fig. 4.



Figure 4. Lift-Plus-Cruise Urban Air Mobility Reference Vehicle. [3]

The model includes estimates for the acquisition, energy, maintenance, infrastructure, and piloting-related costs associated with the aircraft and its operation. We assume piloted operations (i.e., non-autonomous) across a notional number of flight hours per year throughout a notional infrastructure network. Although the analysis did not include other levels of autonomy (e.g., remotely piloted, autonomous), the aircraft are presumed to include automation to reduce pilot workload and help assure safety. The automation integrated into the aircraft is accounted for in the acquisition cost of the aircraft. Additionally, the pilot salary assumed for this analysis was the national average of a non-scheduled transport pilot at 107,780 USD in 2024 [25]. The airframe is assumed to last 10 years and cost 60 USD in maintenance per flight hour. The energy costs are based on the energy capacity of the aircraft; a notional battery energy reserve of 20%; average trip length; and energy unit cost estimates in USD per megajoule [23]. The infrastructure cost is limited to landing and parking fees associated with the weight and class of the aircraft [22]. Refer to Refs. [23] and [22] for additional model details. Future operators will incur additional costs related to indirect costs (e.g., marketing, ticketing, asset management, IT, etc.); however, those costs are not accounted for in this analysis for simplicity. The impact of icing was modeled as a reduction in the yearly flight hours by a given percentage informed by the knock-down factors found in the previous analysis illustrated in Figs. 1 and 2.

Figure 5 shows the potential direct operating cost (DOC) savings possible for average trip lengths of 25 and 50 nautical miles if an anti-icing material could enable all flights assuming that 20% of flights would be impacted by icing. This 20% of icing-impacted flights represents the largest value observed above, so these results provide an estimate on the high end of expected DOC savings. As can be seen in Figure 5, the DOC savings increase as the average trip length grows, and DOC savings are around 2% to 3%. Since our modeling does not include any cost increase for the anti-icing materials, the few percent of DOC savings from increased operations would likely need to offset the increase in costs for such anti-icing materials to be logical to include on UAM aircraft.

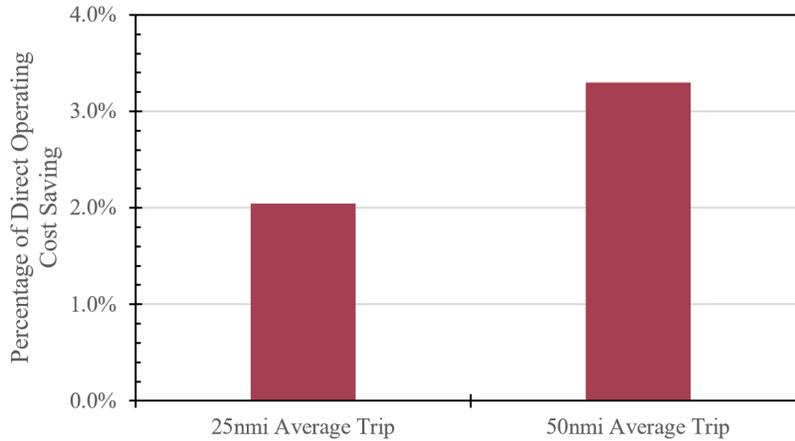


Figure 5. Percentages of estimated direct operating cost savings for notional 25 and 50 nautical mile average trips. The percentages represent the threshold of savings available with anti-icing materials that are capable of enabling 20% of flights that would otherwise have been canceled due to icing conditions.

2.3 AAM Business Viability for Structural Adhesion

Structural adhesion resides on the opposite end of the adhesion spectrum from low-ice-adhesion materials since materials are bonded together rather than experiencing reduced adhesion. Potential advantages of structural adhesion include potential weight savings, reduced manufacturing complexity, and increased production rates, which motivate exploration of their viability for AAM aircraft. We explored AAM business viability of structural designed adhesion in terms of potential unit production cost savings and any insight on break-even points using the developed approach. The approach leverages cost estimation relationships from a modified DAPCA-IV model [26] [4] with an avionics cost model from Gudmundsson [5] and other modifications for eVTOL applications based on engineering intuition and publicly available cost figures [27] [28] to understand reasonable technology scale factors and cost impact bounds for integrating structural adhesive technologies into AAM aircraft. The model was calibrated with publicly available cost figures from current eVTOL developers [27] [28] to ensure the results are within reasonable orders of magnitude prior to applying the technology scale factors. The technology scale factors provide model flexibility to investigate varying levels of cost impact across different cost elements. Model flexibility is an important capability because it enables end-users to tune the cost estimation model for any advanced technology. The approach models a notional structural adhesion alternative as technology factors that modify baseline model parameters by one to five percent applied to various cost factors and the empty weight. The assumption to cap the technology scale factors for a notional structural adhesion at one to five percent is based on engineering intuition and limited manufacturing insight; if experiments are conducted, improved estimates of these parameters can be obtained. The model requires aircraft inputs (empty weight, maximum flight speed, battery capacity, installed power, number of rotors/propellers, diameter of

rotors/propellers, and power absorbed by the rotors/propellers), production inputs (production quantity over five years, Q , and the number of flight test articles), economic inputs (a cost escalation factor to measure inflation and a profit margin) and technology scale factors that adjust the empty weight and baseline estimates for engineering, tooling, manufacturing, quality control, development support, flight testing, and materials costs due to the new structural adhesion technology.

The analysis relied on multiple runs of the cost estimation model to inform rough orders of magnitudes of the cost incurred by integrating advanced technologies. The cost estimation accounts for the research, development, test, and evaluation (RDT&E) and production costs to predict unit costs and purchase prices. The RDT&E and production cost include engineering, manufacturing, tooling, manufacturing materials, development support, flight testing, quality control, and consumables (e.g., electric motors, propellers, rotors, avionics, interior, and battery). The unit cost is determined by dividing the gross RDT&E and production cost by the production quantity over a five-year period.

A notional eVTOL aircraft with integrated designed adhesion technology is modeled with the presumed cost impacts given publicly available information, team insight, and engineering judgment. We assume that integrating designed adhesives would reduce the number of fasteners, require fewer quantities of materials, and streamline manufacturing and tooling due to reduced complexity. These assumptions translate to reductions in structural empty weight and costs related to manufacturing, tooling, and materials. Further, we assume that integrating designed adhesives requires additional cost to engineering, development support, flight testing, and quality control because of the innovative nature of the technology. These increases are based on assumptions that integrating the technology will increase the engineering required to support design decisions; the number of specialized training and personnel to perform the integration will increase; the amount of flight testing to ensure flight loads and performance are maintained across varying flight cycles will increase; and there will be increased quality control necessary to verify adhesive uniformity and adherence to design standards.

As previously, we assume the lift+cruise UAM reference vehicle as the baseline and set the design characteristics and performance inputs to the models based on this aircraft [3]. We study varying production inputs of Q from 10 to 200 aircraft over five years. Assumed other model parameters are three flight test articles; economic inputs for a 2012 to 2024 cost escalation factor (CEF)⁴ and 20% profit margin; and the following technology scale factors: 5% decrease in empty weight, 5% increase in engineering cost, 5% decrease in tooling cost, 5% decrease in manufacturing cost, 5% increase in quality control cost, 5% increase in development support costs, 5% increase in flight test costs, and a 5% decrease in materials costs. The cost escalation factor is required to convert 2012 dollars to 2024 dollars, accounting for inflation.

Figure 6 illustrates the unit cost breakdown for a notional eVTOL with and without designed adhesion technology for a production rate Q of 200 units per year for five years. The modeling estimates the baseline eVTOL would cost nearly 300,000

⁴The baseline model outputs costs in 2012 U.S. Dollars.

USD⁵ per aircraft, while a notional eVTOL with designed adhesion technology could cost approximately 295,000 USD per aircraft.

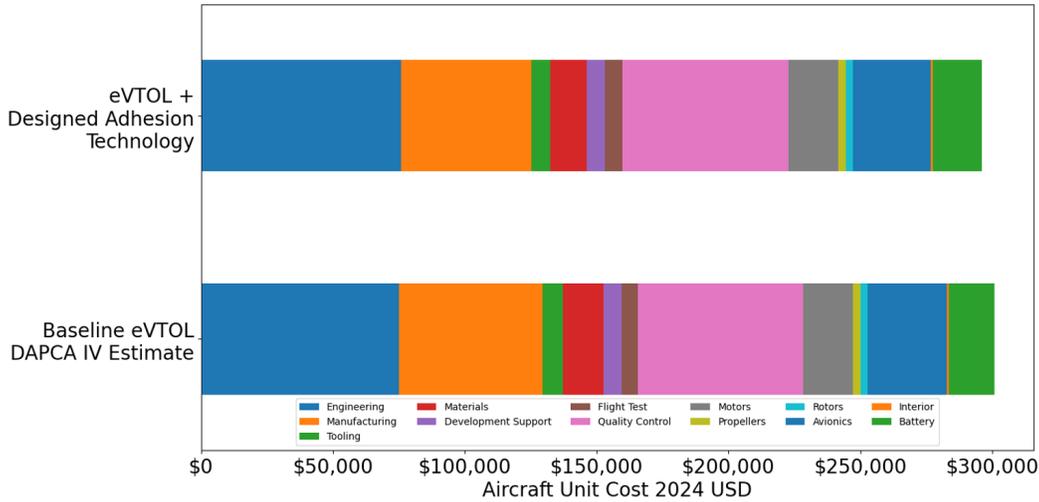


Figure 6. Estimated cost breakdown and comparison of a baseline eVTOL aircraft and a notional eVTOL aircraft integrated with designed adhesion technology using an adapted version of the modified DAPCA-IV cost estimating relationship model [4] [5].

The analysis indicates a 1.6% reduction in the eVTOL aircraft unit cost between the baseline and an aircraft with designed adhesion technology, which results in an estimated cost savings of 4.6M USD over five years. Though the modeling results in lower cost estimates, there is a high degree of uncertainty in assumptions and input parameters, which need to be verified and updated as research into these designed adhesive materials progresses.

To understand the cost impact that the potential increase in production volume enabled by such adhesives may have, we explore the estimated selling price across various productions rates over five years. Since these adhesives may increase production rates, we analyze up to 2,000 units produced over five years—two times the notional production rate. Figure 7 illustrates the unit selling price for a given number of units produced over years on the primary x-axis (on the bottom of the figure) and per month on the secondary x-axis (on the top of the figure). Assuming a 20% profit margin and no spares, the estimated unit selling price of the baseline eVTOL aircraft ranges from 2.9M USD at a production run of 50 aircraft over five years down to 360,000 USD with a production rates of 1,000 units over five years. Similarly, for the notional eVTOL with designed adhesion, the estimated unit selling price ranges from 2.8M USD down to 350,000 USD across the same production rates.

The analysis indicates roughly a 1.8% average reduction in the selling price up to 1,000 units produced over a five-year period for the notional eVTOL integrated

⁵All cost values listed in this section are in 2024 U.S. Dollars (USD).

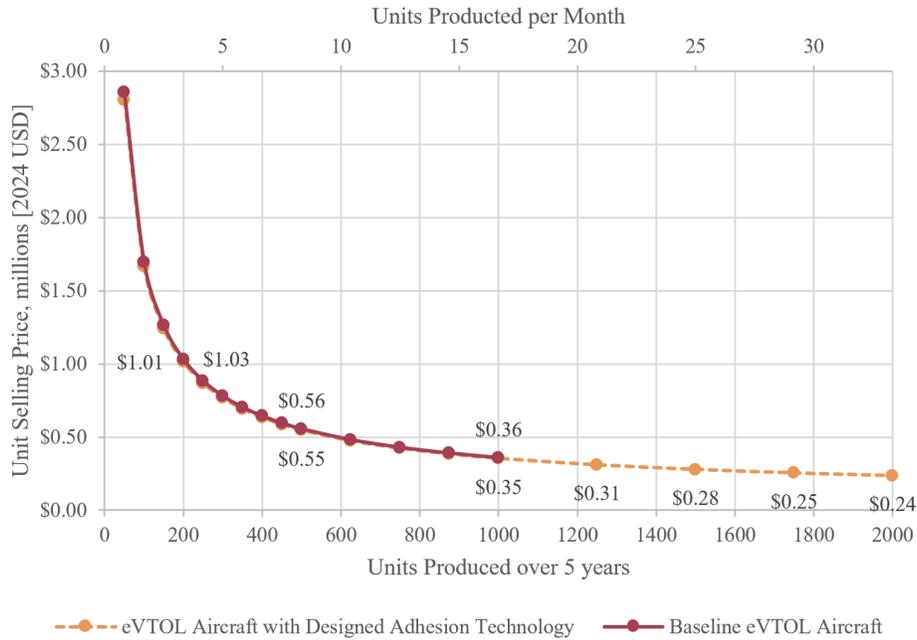


Figure 7. Unit selling price estimates as a function of the units produced over time for a baseline eVTOL aircraft and a notional eVTOL aircraft integrated with designed adhesion technology. The figure includes data callouts for the baseline (upper) and eVTOL aircraft integrated with designed adhesion technology (lower) for reference. The production rates for the notional eVTOL with designed adhesion technology are modeled up to 2000 units produced over five years to estimate the cost impact of increased production rates over the baseline due to the adhesion technology.

with designed adhesion technology. With these selling prices, a manufacturer would lose an estimated 5.6M USD in revenue over five years producing the aircraft made with the designed adhesion technology compared to the baseline aircraft if 1,000 units of each were sold; however, the manufacturer would save 4.6M USD in its own production costs over the same timeframe, leading to a lower gross profit of approximately 1M USD. For the manufacturer to achieve the same gross profit for the new aircraft with designed adhesion technology as the baseline eVTOL aircraft, additional units would need to be produced over the same five-year time period, which should be possible with the new technology. To determine the necessary production run to reach the same gross profit, Figure 8 illustrates the gross profit to the manufacturer for the baseline eVTOL aircraft and the eVTOL with designed adhesion technology; the baseline eVTOL aircraft is assumed to be capped at 1,000 units over five years while the eVTOL with designed adhesion technology is shown for production runs of up to 2,000 units. As can be seen in the figure, if the new technology enables nine additional aircraft per year to be manufactured (for a total of 1,045 units over five years), the manufacturer will generate approximately the same gross profit as in the baseline case. This “breakeven” point sets a likely

minimum target for the necessary production rate increase for the new technology to be advantageous to the manufacturer (based on the assumptions of the analysis). If production can be increased even further and these additional aircraft can all be sold, the manufacturer can generate even greater gross profits.

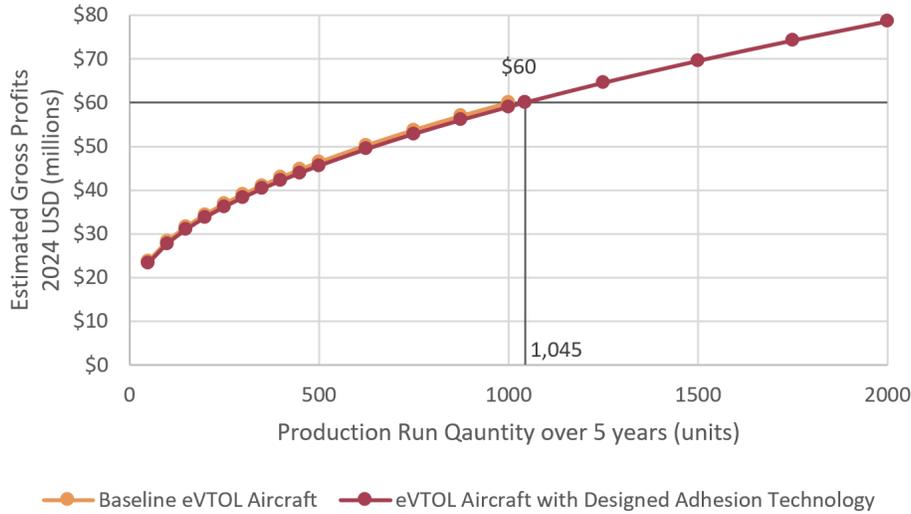


Figure 8. Estimated gross profits of the baseline eVTOL and the eVTOL integrated with designed adhesion technology with an estimated “breakeven” point superposed in black at approximately 60M USD at 1,045 units. The 1,045 units translate to nine additional aircraft per year over five years. The eVTOL aircraft with designed adhesion technology is estimated to outpace the gross profit of the baseline eVTOL aircraft if the technology enables higher production rates.

2.4 Summary of Potential Benefits to AAM

The analysis presented above motivates further exploration of the designed adhesion concept for structural adhesion and low-ice adhesion technologies for Advanced Air Mobility applications. Low-ice adhesive materials could benefit Urban Air Mobility operations by enabling year-round flights. We analyzed previous studies to estimate the expected number of flights impacted by icing and icing-related weather and calculated approximate direct operating cost savings possible by enabling aircraft to operate these icing-impacted flights. Icing and icing-related weather are predicted to impact operations across locations with humid sub-tropical and cold climates by approximately 2% and 20%, respectively. This order-of-magnitude difference has notable impacts on the importance of the technology based on the desired location of operation, i.e., anti-icing technologies are significantly more useful in cold climates. For low-ice adhesion technologies to be economically viable, the cost of these low-ice adhesion technologies should likely be less than three percent of the aircraft’s direct operating cost based on our analysis. With these anti-icing materials, the number of enabled operations could number in the hundreds or tens of thousands of flights

per day for a particular metro area, causing more people and goods to travel safely and efficiently year-round.

Structural adhesion technologies may have positive impacts for eVTOL developers. Our analysis of these technologies explored AAM business viability in terms of unit cost savings from technology integration and impacts of varying production volumes. The modeling of a structural designed adhesion technology with notional technology scale factors indicates an estimated 1.6% reduction in unit cost between a baseline eVTOL and an eVTOL integrated with designed adhesion technologies at a production rate of 1,000 units over a five-year period. The reduction in unit cost by integrating a notional designed adhesion technology translated into an estimated cost savings of 4.6M 2024 USD over the five years given assumptions of technology improvements, production quantity rates, and that eVTOL developers could sell all aircraft produced at a 20% profit margin. Although the estimated unit selling price for the baseline eVTOL would bring in 5.6M USD more revenue than the eVTOL with designed adhesion technologies, the analysis estimates that the designed adhesion technology would “break even” with the baseline aircraft in terms of gross profit generated if the technology could enable an increased production rate of nine aircraft per year over five years. The gross profits could grow well beyond the break-even point if production rates could be increased further. If production rates of 2,000 units (twice the baseline case) could be realized with the new technology, profits could grow by approximately 32%, from 60M USD for baseline eVTOL aircraft to approximately 79M USD with integrating the designed adhesion technology. It is still uncertain if such estimates are realizable with the assumptions and methods required to represent the technology, and the analysis would benefit from additional modeling, analysis, and research to further quantify elements in this study as more is learned about the impacts of the designed adhesives.

3 Low Ice Adhesion Material Design and Evaluation

3.1 Computational Design

Recent advances in the field of molecular simulations have significantly improved our understanding of ice-substrate interactions. These studies are motivated by the need to mitigate ice accumulation on aircraft surfaces, an important aspect for flight safety and operational performance. In particular, molecular dynamics (MD) simulations have become indispensable for elucidating the fundamental mechanisms underlying the formation of the quasi-liquid layer (QLL) at the ice-substrate interface, as well as the nucleation of ice itself. The characterization of the QLL is of particular interest, as this interfacial layer of non-frozen water can act as a lubricating medium that lowers ice adhesion strength, thereby enhancing the anti-icing performance of the substrate. These insights offer a foundation for the rational design of next-generation icephobic coatings. This section highlights the MD studies that examine synthetic polymers and surface treatments developed for anti-icing applications.

Most prior MD works addressing ice-substrate interactions have mainly focused on metallic or idealized flat surfaces [29] [30] [31] [32] [33] [34]. More specifically, MD

simulations have extensively explored interfacial premelting and ice adhesion characteristics on atomically smooth and rigid metallic substrates, elucidating fundamental mechanisms of ice formation, rupture, and adhesion strength at the nanoscale. These studies have highlighted that increased substrate hydrophilicity and structural rigidity tend to reduce ice adhesion, primarily by promoting the formation of thicker and more stable QLLs at the interface. These QLLs act as lubricating barriers that hinder ice-surface binding, a phenomenon also proposed experimentally, [35] thus offering a foundational framework from which studies on polymer-based surfaces have subsequently evolved.

The role of polymer hydrophilicity and chain mobility on ice adhesion characteristics has also been explored with MD-based simulations. For example, Skountzos et al. [6] employed detailed all-atom MD simulations to investigate and compare ice adhesion characteristics on graphite, boron nitride (BN), and cross-linked epoxy polymers. The findings revealed the formation of a QLL at the ice-substrate interface, which, as previously noted, acts as a lubricating layer that effectively reduces ice adhesion strength. The polymer substrate showed a thicker QLL compared to the flat, inorganic crystal substrates (Fig. 9); moreover, this result was attributed to hydrogen bonding interactions between interfacial water molecules and the polymer’s polar groups (especially the hydroxyl moieties), which disrupted the ice crystal structure. This effect was further enhanced by the rough surface texture of the polymer compared to flat crystal surfaces of BN and graphite. Indeed, Uchida et al. [36] demonstrated through MD simulations that increased surface roughness promotes the formation of thicker QLLs, as surface irregularities enhance structural disorder and disrupt the continuity of ice crystals at the interface. Their findings confirmed that amorphous (rougher) silica surfaces induced thicker QLLs compared to crystalline (smoother) surfaces, underscoring the critical role that surface topography plays alongside chemical interactions in optimizing anti-icing performance.

Similar conclusions regarding the QLL formation were also reported by Sato et al., [37] who conducted MD simulations to investigate polymer-based interfacial premelting. They showed that polymer hydrophilicity significantly affects the thickness of the formed QLL, with hydrophilic polymer interfaces such as poly(vinyl alcohol) (PVA) and poly(ethylene oxide) (PEO) promoting thicker and more pronounced QLLs compared to hydrophobic surfaces like polystyrene (PS). The QLL formed by hydrophilic surfaces exhibited reduced mobility. Together, these conclusions provide valuable insights into optimizing polymer surface chemistry to maintain stable premelting layers that effectively reduce ice adhesion.

Several MD studies have focused specifically on PVA, a well-known synthetic analog to antifreeze glycoproteins, and shed light on its mechanisms of ice growth inhibition. Weng et al. [38] for example, demonstrated that the stereochemical compatibility between the hydroxyl groups of PVA chains and the oxygen atoms of the ice lattice underpins its adsorption onto multiple crystallographic planes of ice. Moreover, their results also emphasized the importance of polymer molecular weight (MW), with longer chains more effectively hindering ice propagation. Earlier, Naullage et al. [39] provided computational evidence that the distance between adjacent hydroxyl groups along the PVA backbone closely matches that of surface water molecules in ice, facilitating the alignment of PVA along the ice surface in

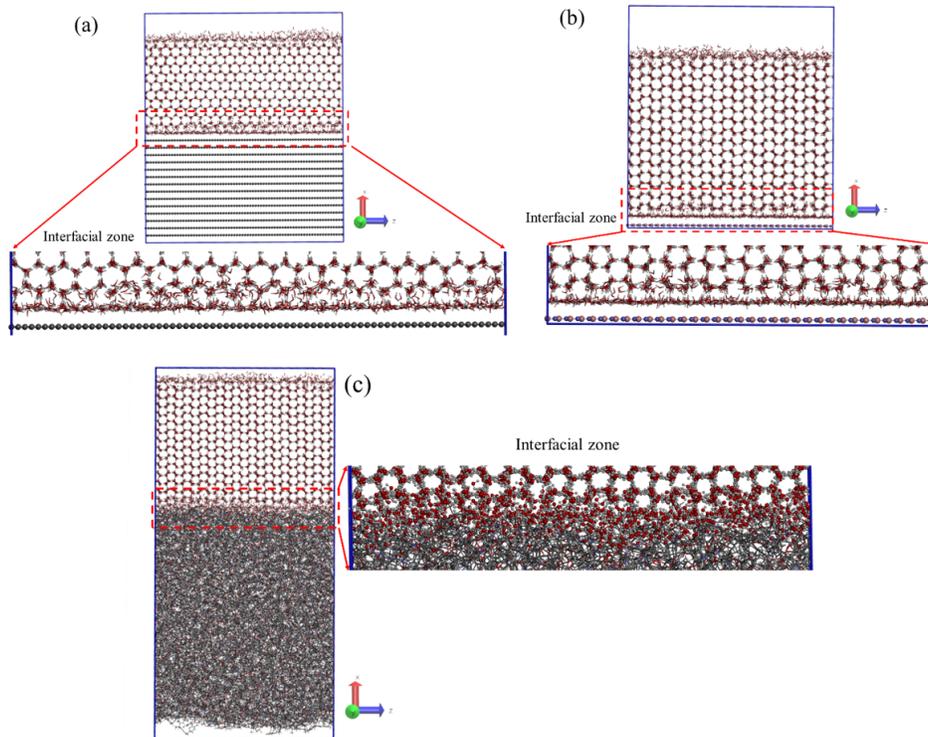


Figure 9. Representative atomic configurations of: (a) graphite/ice, (b) BN/ice and (c) epoxy/ice systems, as obtained from MD simulations. Reprinted with permission from Ref. [6]. Copyright 2024 American Chemical Society.

an extended conformation. Later, Bachtiger et al. [40] advanced the understanding of the stereoselective adsorption behavior of PVA at the ice-water interface, by revealing preferential interactions with primary prismatic ice faces and by highlighting the importance of hydrogen bonding dynamics. More recently, Su et al. [41] combined NIR spectroscopy with MD simulations to investigate the roles of both PVA's hydrophilic (-OH) and hydrophobic (-CH₂) moieties in the inhabitation of ice. Their simulations showed that not only do -OH groups mediate direct binding to the ice lattice via one or two hydrogen bonds, but also that CH₂ groups contribute through hydrophobic interactions with the interfacial water structure. Collectively, these studies emphasized the fact that the dual presence of spatially distributed hydroxyl groups and flexible hydrophobic linkers enables PVA to interfere with ice lattice propagation through both stereochemical matching and interfacial structuring mechanisms, rendering PVA as a prototype system for biomimetic anti-icing polymers.

A study by Smith et al. [42] at NASA investigated silica surfaces functionalized with methyl- and hydroxyl-terminated silane groups. The MD simulations concluded that chain mobility influenced ice adhesion more significantly than terminal chemical functionalities. Longer-chain silane molecules generated pockets of increased free volume, enhancing thus local molecular mobility and disrupting ice's

crystal structure at the interface.

In summary, these investigations reveal three fundamental design principles for advanced anti-icing coatings: (1) enhanced polymer hydrophilicity promotes thicker, more stable QLLs that reduce adhesion, (2) molecular mobility at the interface, tunable via polymer MW and architecture, dictates interfacial layer structure and resilience, and (3) chemical heterogeneity, including functionalized self- assembled monolayers, enables precise control over water-surface interactions. Looking ahead, the advancement of multiscale computational frameworks that bridge atomistic-level insights with macroscopic ice adhesion measurements will be essential for translating MD-based findings into viable, real-world anti-icing technologies.

3.2 Experimental Evaluation

3.2.1 Background

When it comes to assessing the results from ice adhesion measurements, either for bare substrates or coating evaluation, it is critical to understand the ice formation method used. By changing the ice formation method, it is possible to increase or decrease the reported adhesion value by roughly a factor of four [43]. In the published literature, there are three commonly used techniques for producing ice: bulk water ice, precipitation ice, and impact (in-cloud) ice. Bulk water ice is the most extensively tested type of ice since the only piece of equipment required to form it is a climate-controlled chamber or cold room. Formed by placing water inside of molds, this ice can be easily generated in a large number of geometries for testing. Moving towards more involved ice formation processes, the ice that produces the strongest bond with the substrate is precipitation ice, which is formed by super cooled water droplets impacting a substrate in a cold room. The only forces propelling the droplets forward are any pressurized air used in the droplet generation process and gravity. These cold room set-ups are capable of modulating critical factors in aircraft icing such as the liquid water content and median volumetric diameter, both of which influence the adhesion strength. Impact ice, also known referred to as (in-cloud) ice is generated in specialized icing wind tunnels which entrain the droplets within the air flow before impacting the test specimen. While this is this type of ice is the closest to the ice that is generated when aircraft encounter icing conditions, it is also the least commonly tested due to the limited number of facilities that can produce calibrated icing clouds. Facilities can range from small scale tunnels such as the Iowa State Icing Research Tunnel to facilities that can test near flight scale components such as the NASA Glenn Icing Research Tunnel (IRT), however only a handful of calibrated wind tunnels exist in the United States. Within NASA, impact ice has historically been the primary ice type used, with precipitation ice used only to do initial coating assessment. In recent years, bulk water ice has been relegated to early experiment design and the results from this work has not been published.

Unlike other established testing fields, such as material characterization or fracture testing, there are no published standards or recommended practices for conducting ice adhesion testing. This has led to each research group developing a

unique method/geometry for determining the adhesions strength of the ice they generate. While geometry of the test configuration and the method for applying load to the samples can vary wildly based on experimental capability, the three primary means for measuring ice adhesion as a critical stress value are the push test, icing centrifuges, and the modified lap shear test. Currently all three of these methods calculate the ice adhesion strength as the maximum applied force divided by the contact area between the ice and substrate. While the most universal of the test methods and typically used with bulk ice, the push test offers the most variables when it comes to experimental configuration. It has been shown that factors such as sample size, loading location, strain rate, and substrate thickness can significantly influence the reported adhesion strength with the interplay between these experimental parameters causing a wide range of results for what should be the same material system. As the field of ice adhesion advanced, a more specialized icing test was designed which imitates the forces applied to ice accreted on rotating components. Known as centrifuge testing, there are several different variations that have emerged over the years based on the capabilities available of each research group [44]. Due to the additional complexity of instrumenting rotating equipment which spins at hundreds to thousands of revolutions per minute, it is not achieved the widespread adoption of the push test. A relatively quick testing method to conduct, it enables the rapid screening of low ice adhesion coatings at the Anti-Icing Materials International Laboratory (AMIL) at the University of Quebec at Chicoutimi, National Research Council Canada (NRC), Adverse Environment Rotor Test Stand (AERTS) at Penn State University, and NASA Langley. The final adhesion test that is commonly used is the modified lap shear test, which has been the primary measurement technique used at NASA Glenn. Seeking to replicate more mature materials testing, this method requires significant hands-on work from the researcher to run, but still has the ability to have very high throughput. Using samples generated at the NASA Glenn Icing Research Tunnel, both sides of the sample are secured before testing to eliminate any unintended forces along with a rigorous set of testing procedures which is designed to reduce scatter in the data set.

While there are a plethora ice adhesion test methodologies available, it is rare for a single research group to have access to more than a couple of methods. Due to the significant differences in test set-ups and ice types available to given research groups it is extremely difficult to make direct comparisons, either between or against ,published data. Several attempts have been made to better understand the differences between experimental set-ups, with two large interfacility comparison tests being conducted in recent years. The project lead by Ronneberg showed that agreement in both absolute value of the adhesion strength and data trends is possible [45]. However, this was not the case in the expanded interfacility comparison study lead by Rehfeld, which included results from 13 research groups using a variety of methodologies [46]. Despite strict controls on the substrate preparation and coating procedures, the adhesion results between the facilities showed significant differences in both absolute value and trend. For one of the adhesion tests done using a substrate coated in PTFE-Tape, one group reported an 80% reduction in adhesion strength compared to a bare substrate while another measured a 70% in-

crease in adhesion strength against the same case. This highlights one of the largest issues that currently exists in the ice adhesion community, where while published data is plentiful, the ability to compare experimental results is extremely difficult and for almost all cases impossible. Lastly, due to the inability to strictly control the ice formation process, it is not uncommon for the reported standard deviations of the adhesion measurements to be on the same order of magnitude as the reported adhesion strengths [47].

3.2.2 Ice Adhesion Testing at NASA

The primary test method used by NASA to measure the ice adhesion strength to both bare and coated substrates is the modified shear lap joint test located at NASA Glenn Research Center [48]. Samples for this test are generated by placing small coupons into the NASA Glenn Icing Research Tunnel on which impact ice is generated before removal from the tunnel and mechanical testing. Both the samples in the IRT as well as the custom test set-up located inside of a climate-controlled chamber are shown in Fig. 10. Using a peak-load analysis method, the adhesion strength can be quickly determined for an individual sample and the enough data can be swiftly processed to form statistical models of ice adhesion trends as they relate to icing conditions. Additionally, NASA has two ice adhesion centrifuges, the AERTS Jr. I (AJ1) located at NASA Langley and the AERTS Jr. II (AJ2) at NASA Glenn. Used extensively in screening tests for potential low ice adhesion coatings, AJ1 tests against precipitation ice inside of a cold chamber [49]. Based on lessons learned from the construction and operation of AJ1, the newer AJ2 centrifuge is currently located in a cold chamber and was designed with the potential for future operations inside of the IRT. It is capable of being operated completely hands-free which helps prevent any damage to the sample along with the ability to accurately control the acceleration / strain rate of the experiment. Using a modular coupon system, AJ2 is capable of rapidly testing a variety of coatings and is one of the few centrifuges that contains design considerations for testing inside of an icing research tunnel, with the only other known example being the centrifuge rig located at NRC in Ottawa, Canada.



Figure 10. Modified lap joint shear samples in the IRT (left) and experimental lap shear apparatus (right).

Besides the operational capabilities of both the IRT and adhesion testing rigs,

NASA also home to several additional experimental measurements which can improve the ability to interpret ice adhesion test results. The first is the implementation of digital image correlation (DIC), it is possible to accurately measure the surface displacements of a sample undergoing testing using the modified lap shear test. From this, the interfacial stresses and strains can be calculated along with a direct simulation of the experiment numerically [50]. An additional technique available at NASA Glenn is the ability measure the grain size of impact ice using a custom machine learning algorithm [51]. An example of the process where an image of the ice is via an optical microscope, initial boundary identification via machine learning is conducted, the boundary closure procedure to produce individual grains and an overlay with the optical image to ensure accuracy is shown in Fig. 11. Using this, the changes in ice grain size can be characterized as different substrate and icing conditions are tested. These additional data points provide an extra layer of detail pertaining to both the material being tested as well as the mechanics of the experiment that is not available to samples tested at other institutions.

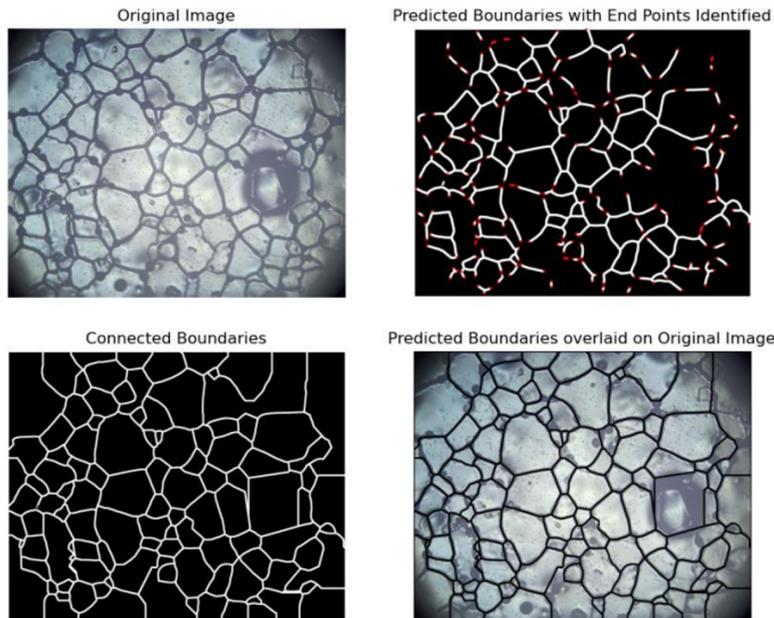


Figure 11. Process for automatically determining grain boundaries via machine learning.

4 Structural Bonding

Adhesive bonding has been used in aircraft structures and interiors to join components for many decades and rapidly replacing or supplementing traditional mechanical fasteners, which offer benefits including reduced weight, mitigating stress concentration, improved corrosion resistance, better mechanical/acoustic damping, smoother surface for better aerodynamic performance, and broadening design space

for complex geometry especially for rapidly evolving diverse advanced air mobility (AAM) vehicles for both passenger and cargo transport. NASA pioneered development of structural adhesives and sealants since the 1980s for potential application to high-temperature, high-speed transports under High-Speed Research (HSR) (High-Speed Civil Transport (HSCT)) program [52]. Reliable structural adhesives enable high-rate aircraft manufacturing, unitized structures, automation, minimizing part count and fasteners, which all contribute to increasing production rates and reducing weight and cost to meet growing demand in AAM market as well as conventional commercial and military aviation [53]. It is desirable that structural adhesives offer reliable and sustainable bonding with various adherends (composites, metals, thermoplastics, and so on) to eliminate or minimize time-consuming drilling and heavy mechanical fastening to provide complex design space and rapid production rate for the rapidly growing AAM market. In addition, there has been a growing interest in the development of lightweight adhesives from renewable, sustainable, and recyclable resources to increase efficiency and profitability.

Structural adhesives can be viable owing to the growing worldwide demand to double aircraft production rates within next 20 years. This demand comes from commercial aircraft to meet rapidly increasing personal and business travel as well as the emerging AAM market. Improving structural adhesives is expected to help increase production capacity by alleviating part count and fasteners, thus reducing assembly rate, time, and weight. In addition, structural adhesives offer a more flexible design space to adapt new materials and processes to the emerging AAM market. Early success of commercialization of high-temperature structural adhesives developed for the NASA HSR program can guide a viable lesson to create a sustainable US supply chain through public-private partnership. NASA LaRC PETI (phenylethynyl terminated imide) series adhesives developed for high-temperature resin and adhesives under the HSR program was commercialized and selected as the NASA Commercial Invention of the Year [54].

The strength of structural adhesives is to improve the production rate because time-consuming drilling and fastening processes are eliminated or minimized, which allows to customize new additive manufacturing processes and continuously evolving AAM vehicle design efficiently. Weight reduction (15% for a wing box) of lightweight structural adhesives by eliminating fasteners and thinning components can improve fuel efficiency while minimizing greenhouse emission [55]. Elimination of holes and fasteners for composites can save assembly cost and time and mitigate stress concentration while improving vibration, shock, and fatigue resistance.

Conventional thermoset adhesives are not repairable and recyclable, which is a drawback compared with the mechanical fasteners. Newly developed thermoset polymers such as vitrimers [56] and dynamic bonding thermosets [57] [58] can overcome the limited repairability and recyclability via thermally activated reversible bond-exchange reactions. Thermoplastic polymers and composites also have been used over the past decades as prepeg tapes and adhesives because of the economic advantages associated with reduction of scrap, near infinite shelf life, reusability, repairability, reduction in manufacturing equipment investment, higher rates of production from tape to part, and increased structural customization. Recently, structural adhesives based on biological source materials have been developed, which

exhibit lap shear strength as good as industrial epoxy adhesives [59] [60]. The renewable natural resources come from current crop plants and are abundant with a cost that is comparable to epoxy monomers. Although encouraging, biologically sourced adhesives would need similar vetting as the high-temperature structural adhesives developed for the HSR program, which were shown to have structural integrity even in harsh flight environments such as elevated temperatures and extended hot-wet conditions [52].

Reliable and sustainable performance of structural adhesives need to be certified and qualified based on quantitative testing data. However, standard methods need to be adopted for newly developed additive manufacturing parts to ensure AAM vehicle safety. Moreover, advanced real time nondestructive evaluation (NDE) techniques and in-situ monitoring tools need to be developed as well to evaluate reliability and life of structural adhesives precisely and timely for rapid certification. Improvement of integrated streamlined relationships in aircraft design, materials, certification, and manufacturing methodologies is essential to successful structural adhesive development to improve production rate and environmental impact.

5 Bio-engineered Adhesives

5.1 Bioengineered Polymer Design

Biological systems contribute to the fundamental understanding of anti-icing and adhesion, which has been translated to the production of new types of adhesives and coatings. Prior to the advent of synthetic polymers, adhesives were produced from biological sources such as animal collagen or cereal gluten proteins [61]. Traditional, biologically derived glues are water soluble and do not have the adhesive properties needed for aerospace applications. However, the evolutionary trajectories of individual species in the tree of life have solved different adhesion problems to adapt to specific ecological niches.

Marine invertebrates such as barnacles, mussels, and sandcastle worms produce protein adhesives that form strong bonds in marine environments [62]. Biochemical analysis of marine glue proteins from barnacles, mussels, and sandcastle worms revealed common mechanisms in which multiple hydrophobic glue and self-assembling amyloid fibril or non-amyloid fiber proteins are secreted independently and mixed in the marine environment with pH and salinity changes driving curing [63] [64]. These marine adhesive proteins are essentially a hydrophobic polymer to provide cohesion with amino acid copolymer subunits that provide the adhesive force. For mussels and sandcastle worms, the adhesive force comes from many of the tyrosine amino acids in glue proteins being post-translationally modified to DOPA. By contrast, the primary protein sequence of barnacle cement proteins is sufficient to provide adhesion [65]. Intriguingly, barnacle cement proteins have similar primary protein sequence motifs as spider silk proteins [66]. Spider silk is another example of a natural adhesive protein that is being investigated for commercial use [67].

Proteinaceous adhesives have also been identified from frog, snail, slug, and velvet worm species [68]. Snails and slugs can produce an adhesive mucus that is dependent upon interactions of positively charged glue proteins with negatively

charged polymers [69]. Although the biochemical mechanisms driving adhesive properties for frogs and velvet worms are not as well understood, the adhesive proteins found in *Notaden bennetti* frogs and *Euperipatoides* sp. velvet worms have similar amino acid composition and encode intrinsically unstructured proteins [70]. Thus, there are multiple examples of convergent evolution of adhesive protein sequences between more distantly related animal species. These similar primary sequence motifs suggest there a limited number of chemical mechanisms to evolve adhesive proteins from biological amino acids. However, nature has not fully explored the biological adhesive chemical space. The mechanistic insights from biological adhesive proteins have been broadly applied to generate synthetic proteins, bio-inspired synthetic adhesives, and biologically sourced adhesives.

Synthetic biology allows researchers to test proteins that do not exist in nature and to investigate a greater range of chemical composition in biologically produced macromolecules. Several studies have generated synthetic adhesive proteins based on the repeated amino acid sequence of the Elastin protein. Elastin is a primary component of elastic tissues in a subset of vertebrates and is a polymer of repeated short amino acid sequences [71]. Elastin-like proteins can be produced by repeating five amino acids of Val-Pro-Gly-Xaa-Gly, where Xaa can be any amino acid except proline. Lin and Liu [72] synthesized Elastin-like protein adhesives with either tyrosine or cysteine in the variable site, which were expressed in bacteria. Synthetic protein expression in microbes can be challenging. To produce novel proteinaceous adhesives, Shi et al. [73] chemically synthesized Elastin-like polypeptides. An Elastin-like protein sequence has also been fused to a barnacle cement protein to produce a synthetic protein with up to 4 MPa adhesion on steel [74].

Insights from marine adhesive proteins have also been applied to biomimetic synthetic polymer design. Incorporating DOPA into a carboxyl-containing polyurethane improved adhesion to iron substrates by 30% over the non-modified polyurethane [75]. The adhesive functional group of DOPA is a catechol, and Matos-Pérez [76] tested multiple polystyrene co-polymers with differing ratios of styrene and 3,4-dihydroxystyrene with the latter subunit containing the catechol functional group. Maximal adhesion was observed when 33% of the polymer contained the catechol subunit. These are only two of many examples of incorporating DOPA or catechol functional groups into synthetic polymers to develop adhesives [64].

The diverse chemical properties of biological polymers can also be leveraged as substrates for biologically sourced adhesives using feedstocks from crops. One of these adhesives is made from the corn seed storage protein zein, which is naturally hydrophobic, and mixed with tannic acid derived from plant polyphenols to make an adhesive with lap shear strength similar to super glue [77]. More recently this group showed that epoxidized soy oil combined with malic acid and tannic acid can produce industrial strength adhesives [59]. These biologically sourced adhesives were developed with chemical principles from marine adhesive protein basic research. Specifically, that the adhesive needs a hydrophobic polymer backbone to provide the structural integrity. The hydrophobic polymer is chemically bonded to aromatic functional groups with structures analogous to catechol, which provides the adhesive property. Drawing inspiration from snail glue, Zhu et al. [60] combined positively charged ϵ -poly-L-lysine with negatively charged poly-glutamic acid to generate a

polypeptide glue with adhesive strength of up to 28 MPa on ceramic surfaces.

In addition to adhesion, organisms adapted to cold environments provide potential anti-icing solutions. Organisms adapted to the Arctic or Antarctic have independently evolved ice binding proteins to either become more tolerant to freezing or to inhibit ice crystal formation at subzero temperatures [78]. Freeze tolerance can be conferred by proteins that inhibiting ice recrystallization or through guiding ice crystallization extracellularly. By contrast, antifreeze proteins (AFPs) lower the freezing point of water within the organism by binding small ice crystals to restrict crystal growth. Direct incorporation of AFPs into anti-icing surfaces has been proposed for a variety of engineering applications including aviation [79]. For example, AFPs extracted from cod fish have been incorporated into asphalt and shown to reduce the rate of ice formation at subzero temperatures and decrease ice adhesion to the biohybrid asphalt [80]. Coating a biohybrid asphalt with carbon nanotubes and silicon carbide generates a more durable anti-icing surface [81].

The large diversity of ice binding proteins provides multiple physical and chemical mechanisms that could be leveraged with synthetic biology or biomimetic designs to provide anti-icing solutions for aircraft. For example, Gao et al. [82] generated a novel gene encoding a consensus protein domain from mussel foot proteins and an antifreeze protein domain from the yellow mealworm beetle. Expressing small quantities of the novel protein in bacteria allowed the researchers to measure disruption of ice formation on surfaces coated with the adhesive-AFP fusion protein. Similarly, synthetic peptides containing marine glue DOPA residues and antifreeze protein motifs effectively coated silicon surfaces and reduced freezing temperatures of water ice [83]. A biomimetic graphene oxide nanosheet coating was recently developed using zwitterionic functional groups to mimic the small ice crystal binding function of AFPs [84]. This coating delayed ice formation, reduced freezing temperature, reduced ice adhesion non-functionalize graphene oxide or polydimethylsiloxane coatings.

Finally, organisms have also evolved surface geometries that impact adhesion. Gecko toe pad scales forms an adhesive surface that is primarily due to the microstructure arrangement of the scales [85]. Although the epidermal surfaces of plant leaves and petals are coated by a hydrophobic cuticle layer, microstructures influence wettability [86]. For example, rose petals are adhesive for water, while rice leaves direct water shedding along the leaf. Bioinspired surface textures could alter biochemical adhesion properties as well as impact non-organic surfaces such as metals.

5.2 Role of Modeling and Simulation in Designing Bio-inspired Coating Materials for Aeronautics Applications

Biological and bio-inspired materials offer tunable icephobic and adhesive properties that can be leveraged to develop next-generation coatings. Unlike synthetic materials, proteins and other biomolecules allow for precise control over both substrate interactions and intermolecular forces through sequence-level amino acid modifications. However, this tunability introduces significant design challenges. For instance, a protein with ten active binding residues could theoretically yield about

20^{10} unique combinations, but only a few sequences may exhibit the desired functionality. Moreover, for aeronautics applications, the designed protein must also remain stable under non-native or harsh environmental conditions. To efficiently explore this vast and sparse design space and identify functional, stable variants, molecular modeling and computational design strategies are essential for guiding experimental discovery.

Simulations have played a crucial role in uncovering the ice-binding mechanisms of antifreeze proteins (AFPs), which are often challenging to characterize experimentally. Hudait et al. [87] used multi-resolution MD simulations to study a hyperactive insect AFP, TmAFP. They found that in pre-nucleated solutions, TmAFP recognizes ice via slow diffusion and reorientation to match the lattice structure. They also proposed that the binding is driven primarily by enthalpy gain, as the natural rigidity of TmAFP minimizes entropy loss upon binding. While this work explains how AFPs inhibit ice growth by binding to nucleated crystals, some AFPs exhibit a seemingly paradoxical behavior, enhancing ice nucleation under certain conditions. This contrasting property, previously observed experimentally, [88] was elucidated by Zhang et al. [89] through extensive MD simulations. Their study showed that AFPs can lower the free energy barrier for ice nucleation from a supercooled liquid, by templating water molecules into structured intermediates, progressing from 1D chains to 2D nanosheets and ultimately to 3D ice nuclei (Fig. 12). These works provide molecular design rules, such as leveraging structural rigidity to minimize entropy loss, that can be exploited to optimize AFP performance. In fact, some studies have explicitly applied these principles to predictive design, using simulations to identify structural features linked to antifreeze activity. Kozuch et al. [90] simulated multiple AFPs to extract water dynamics and protein structural features near ice-binding and non-binding surfaces. These features were used to train a neural network that accurately predicted thermal hysteresis activity. Building on this, the authors applied a genetic algorithm to design AFP variants with reduced thermal hysteresis by up to 1.3 K relative to the wild type. [91]

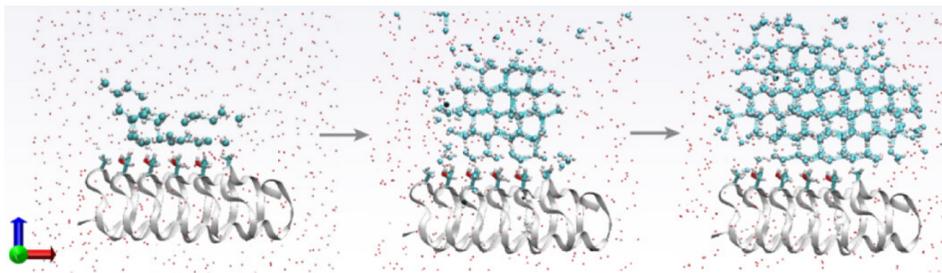


Figure 12. MD simulation evidence of growth of an ice nuclei into a 3D ice nanocrystal on the ice binding surface of TmAFP. The central backbone of the protein is depicted using a silver cartoon representation, while the functional groups on the ice binding surface are highlighted with sticks (C - blue; O - red; H - white). The water molecules in the liquid are represented by red spheres, whereas those in the ice-like layers are represented by blue-white spheres. Image modified from ref. [89] CC BY 4.0.

Molecular modeling has also been instrumental in predicting how biomaterials mediate substrate interactions critical for adhesion. For example, Kumar et al. [92] used molecular dynamics simulations to study the barnacle cement protein MrCP20 interacting with calcite surfaces and $\text{Ca}^{2+}/\text{CO}_3^{2-}$ ions. Their results revealed that no single residue or motif drives surface adhesion. Instead, a combination of charged amino acids and water-mediated interactions enables ion adsorption on the protein surface. This binding is coupled with a disorder-to-order transition in MrCP20, enhancing its structural stability. The study highlights how spatial charge patterning contributes to both mineral binding and adhesion. In a related study, Yeh et al. [93] investigated the adsorption of catechol, a key motif in mussel foot proteins, on hydroxylated (hydrophilic) and non-hydroxylated (hydrophobic) alumina surfaces. MD simulations and free energy calculations showed that catechol binds strongly to both surfaces via distinct mechanisms. In aqueous environments, catechol displaces water to bind hydrophobic alumina directly, while hydrogen-bond networks mediate its interaction with hydrophilic alumina. Under anhydrous conditions, strong binding is observed on both surfaces due to the absence of water competition. Together with earlier studies on catechol adsorption to metal substrates like gold, [94] these findings underscore the value of atomic-level modeling in guiding the rational design of robust, surface-specific bio-inspired adhesives.

Collectively, the studies discussed above provide a strong foundation for the rational design of adhesive proteins and antifreeze proteins, by offering strategies to optimize molecular function for application in coatings. Recent advances in generative AI have enabled rapid exploration of sequence-structure-function relationships for protein design, [95] [96] [97] [98] and these methods can be directly applied to the design of bio-inspired adhesives and icephobic proteins. Beyond functional performance, ensuring the stability of these computationally designed proteins under non-native or operational conditions, such as low humidity, temperature extremes, or mechanical stress is equally important for aeronautics applications. Computational methods are particularly well-suited to address these challenges, enabling predictive screening of stability across diverse environments. This integration of functional design with stability optimization represents a critical and promising direction for future research.

5.3 Potential for Biohybrid Coatings and Adhesives

The significant advancements in bioinspired and biologically sourced adhesives and anti-icing surfaces suggests that they could soon be implemented in aircraft construction and operations. However, protein and biomimetic adhesives and coatings need to remain functional over decades of use in the harsh environmental conditions for aircraft operations and storage including extended exposure to full spectrum sunlight, extreme temperature variations, moisture, abrasion, and physical stresses. Many of the adhesives and coatings discussed above do not have sufficient adhesion force or are not durable for implementation in aviation. For example, catechol-polystyrene is a durable polymer but lacks sufficient adhesion for use as a structural adhesive [76]. By contrast, snail-inspired poly-lysine/poly-glutamic acid glue has remarkable adhesion strength when dry, but adhesion is essentially lost when glued

joints are exposed to moisture [60].

A common challenge in translating protein functions to biomimetic technologies is scaling from protein macromolecules to small molecule polymer chemistry. This approach distills active site chemistry from complex secondary or tertiary protein structures into small functional groups, which requires extensive empirical formulations and trials to identify successful adaptations. By contrast, directly employing proteins as biologically sourced adhesives or coatings into an aerospace technology would allow functions requiring the higher order folding of proteins to be utilized. Unfortunately, proteins absorb moisture, are sensitive to extreme temperatures, and are more readily degraded by microbes.

Potentially, biohybrids that incorporate proteins into traditional materials could shorten the time needed to translate biological mechanisms into biomimetic technologies. Addition of DOPA to polyurethane or fish AFP to asphalt improved adhesion or anti-icing properties relative to the reference materials, respectively [75] [80]. This approach could be expanded to conventional aircraft adhesives and coatings that use epoxies and polyurethanes. Epoxide bonds react with amine and imidazole to harden into epoxy. Every amino acid has an amine that is used to form peptide bonds. Lysine, arginine, asparagine, and glutamine also have amines in their functional groups, while the histidine side chain is an imidazole. Hydroxyl groups react with an isocyanate in the polyurethane reaction. All amino acids have a carboxyl group that includes a reactive hydroxyl moiety. Aspartate, glutamate, serine, threonine and tyrosine all have hydroxyl moieties in their side chains. Thus, the functional groups found in proteins have the potential to allow direct chemical incorporation of short peptides or longer proteins into conventional plastic resins.

6 Discussion

This paper detailed the pre-execution activities of the Designed Adhesion effort in NASA's CAS project. The purpose of the pre-execution activities were to identify Desirability, Viability, and Feasibility (DVF). This was accomplished by narrowly evaluating the impact of designable adhesion on the AAM market.

A review of the state-of-the-art in various regimes on the adhesion spectrum was performed and detailed. Ultimately a detailed workplan was developed for execution that was tailored to the available subject matter expertise at across three NASA centers. That detailed workplan was excluded from this document.

However, one of the main goals of the workplan in all three research areas (low ice adhesion, structural adhesives, and bio-engineered adhesives) was to more closely couple the recent advancements in computational modeling with state-of-the-art experimental measurement techniques to meet two major goals. The first goal is to more fundamentally understand the interfacial physics of adhesion. The second goal is to validate that results of molecular based models can be evaluated in a predictive fashion, even just qualitatively, to determine if a material has desirable adhesive properties.

Due to the large parametric space, as well as the significant cost of fabrication and evaluation of individual materials, a purely empirical approach to adhesive

design is impractical for designing a tailored adhesive solution. Leveraging computations to compliment experimental efforts is a necessity as we move towards the future of aviation.

References

1. Kim, S., Justin, C. Y., and Mavris, D., “Investigation of Weather Considerations for Battery Electric Regional Air Mobility Flights,” *AIAA AVIATION Forum*, 2024, AIAA 2024-3728.
2. Chao, H., Maheshwari, A., DeLaurentis, D., and Crossley, W., “Weather Impact Assessment for Urban Aerial Trips in Metropolitan Areas,” *AIAA AVIATION Forum*, 2021, AIAA 2021-3176.
3. Silva, C., Johnson, W. R., Patterson, M. D., and Antcliff, K. R., “VTOL Urban Air Mobility Concept Vehicles for Technology Development,” *2018 Aviation Technology, Integration, and Operations Conference, AIAA AVIATION Forum*, 2018, AIAA 2018-3847.
4. Raymer, D., *Aircraft Design: A Conceptual Approach, Sixth Edition*, American Institute of Aeronautics and Astronautics, 2018.
5. Gudmundsson, S., *General Aviation Aircraft Design: Applied Methods and Procedures*, Butterworth-Heinemann, 2014.
6. Skountzos, E. N., “Interfacial Characteristics of Ice-Supporting Substrates via Molecular Dynamics Simulations,” *Langmuir*, Vol. 40, 2024, pp. 26864–26874, <https://doi.org/10.1021/acs.langmuir.4c03106>.
7. Garrow, L. A., German, B., Schwab, N. T., Patterson, M. D., Mendonca, N., Gawdiak, Y. O., and Murphy, J. R., “A Proposed Taxonomy for Advanced Air Mobility,” *AIAA AVIATION Forum*, 2022, AIAA 2022-3321.
8. Antcliff, K. R., Moore, M. D., and Goodrich, K. H., “Silicon Valley as an Early Adopter for On-Demand Civil VTOL Operations,” *16th AIAA Aviation Technology, Integration, and Operations Conference, AIAA Aviation*, 2016.
9. Holden, J. and Goel, N., “Fast-Forwarding to a Future of On-Demand Urban Air Transportation,” Tech. rep., Uber, 2016, accessed 3 June 2024.
10. “Vertiport Design, Supplemental Guidance to Advisory Circular 150/5390-2D, Heliport Design,” Engineering Brief 105A, Federal Aviation Administration, 2024.
11. Antcliff, K., “Regional Air Mobility: Leveraging Our National Investments to Energize the American Travel Experience,” White paper, National Aeronautics and Space Administration, 2021.
12. Hackenberg, D. L., “NASA Aeronautics Research Mission Directorate (ARMD) Urban Air Mobility (UAM) Grand Challenge Industry Day,” 2018.

13. Moore, M., Goodrich, K., and Patterson, M., “ODM Technical Roadmap Report Out,” 2016, <http://www.nianet.org/ODM/September/1%20Hartford%20Intro%20Slides%20Goodrich.pdf>.
14. Patterson, M., “Manufacturing, Integrated Structures, and Community Impact (MISC) Working Group Update,” *On-Demand Mobility Roadmapping Workshop*, Arlington, VA, 2016.
15. Maheshwari, A., Mudumba, S., Sells, B. E., DeLaurentis, D. A., and Crossley, W. A., “Identifying and Analyzing Operations Limits for Passenger-Carrying Urban Air Mobility Missions,” *AIAA AVIATION Forum*, 2020, AIAA 2020-2913.
16. Maheshwari, A., Sells, B. E., Harrington, S., DeLaurentis, D., and Crossley, W., “Evaluating Impact of Operational Limits by Estimating Potential UAM Trips in an Urban Area,” *AIAA AVIATION Forum*, 2021, AIAA 2021-3174.
17. Edsel, A., Das Biswas, S., Kilbourne, M., Gadre, R., Vashi, S., Mall, K., Crossley, W. A., DeLaurentis, D. A., Patterson, M. D., and Sells, B. E., “Exploring Ridesharing in Passenger Urban Air Mobility: A Comparative Analysis,” *34th Congress of the International Council of the Aeronautical Sciences*, Sept. 2024.
18. Justin, C. Y., Payan, A. P., Winfield, S. C., Ramirez, L. A. M., and Mavris, D. N., “Combined Passenger and Cargo Operations for Electrified Regional Air Mobility,” *AIAA SCITECH 2022 Forum*, 2022, AIAA 2022-0259.
19. Justin, C. Y. and Mavris, D. N., “Regional Air Mobility Market Study,” *33rd Congress of the International Council of the Aeronautical Sciences*, Stockholm, Sweden, 2022.
20. Justin, C. Y., Payan, A. P., and Mavris, D. N., “Integrated fleet assignment and scheduling for environmentally friendly electrified regional air mobility,” *Transportation Research Part C: Emerging Technologies*, Vol. 132, 2022, pp. 103567.
21. Goyal, R., Reiche, C., Fernando, C., Serrao, J., Kimmel, S., Cohen, A., and Shaheen, S., “Urban Air Mobility (UAM) Market Study Final Report,” Contractor Report NASA HQ-E-DAA-TN65181, National Aeronautics and Space Administration, Nov. 2018.
22. Howard, R., Wright, E. C., Mudumba, S., Gunady, N., Sells, B., and Maheshwari, A., “Assessing the Suitability of Urban Air Mobility Vehicles for a Specific Aerodrome Network,” *AIAA AVIATION Forum*, 2021, AIAA 2021-3208.
23. Kohlman, L. W., Patterson, M. D., and Raabe, B. E., “Urban Air Mobility Network and Vehicle Type—Modeling and Assessment,” NASA/TM—2019-220072, National Aeronautics and Space Administration, 2019.
24. “NASA Urban Air Mobility (UAM) Reference Vehicles,” accessed 13 Aug 2025.

25. *Occupational Outlook Handbook*, chap. Airline and Commercial Pilots, Bureau of Labor Statistics, U.S. Department of Labor, visited 13 Aug 2025.
26. Boren, Jr., H. E., “DAPCA: A Computer Program for Determining Aircraft Development and Production Costs,” 1967.
27. “Commercializing Aerial Ridesharing,” 2021, accessed 19 Aug 2025.
28. Archer Aviation, “Future Flight Global Announces Planned Purchase of up to 116 Archer Midnight Aircraft Worth up to \$580M,” 13 August 2024, accessed 19 Aug 2025.
29. Baran, L., “Understanding Interfacial Ice Premelting: Structure, Adhesion, and Nucleation,” *The Journal of Physical Chemistry*, Vol. 129, 2025, pp. 4614–4631, <https://doi.org/10.1021/acs.jpcc.4c07328>.
30. Chang, Y., “Unraveling Ice-Solid Interface Rupture Dynamics: Insights from Molecular Dynamics Simulations,” *Langmuir*, Vol. 40, 2024, pp. 17090–17097, <https://doi.org/10.1021/acs.langmuir.4c02079>.
31. Metya, A., “Ice Adhesion Mechanism on Lubricant-Impregnated Surfaces Using Molecular Dynamics Simulations,” *Molecular Simulation*, Vol. 45, 2019, pp. 394–402, <https://doi.org/10.1080/08927022.2018.1513649>.
32. Sun, Q., “Quasi-Water Layer Sandwiched Between Hexagonal Ice and Wall and its Influences on the Ice Tensile Stress,” *Nanoscale*, Vol. 14, 2022, pp. 13324–13333, <https://doi.org/10.1039/D2NR02042D>.
33. Sun, Q., “Molecular Dynamics Simulation of Thermal De-icing on a Flat Surface,” *Applied Thermal Engineering*, Vol. 189, 2021, pp. 116701, <https://doi.org/10.1016/j.applthermaleng.2021.116701>.
34. Xiao, S., “Nanoscale Deicing by Molecular Dynamics Simulation,” *Nanoscale*, Vol. 8, 2016, pp. 14625–14632, <https://doi.org/10.1039/C6NR02398C>.
35. Chen, D., “Icephobic Surfaces Induced by Interfacial Nonfrozen Water,” *Applied Materials and Interfaces*, Vol. 9, 2017, pp. 4202–4214, <https://doi.org/10.1021/acsami.6b13773>.
36. Uchida, S., “Structure of the Water Molecule Layer between Ice and Amorphous/Crystalline Surfaces Based on Molecular Dynamics Simulations,” *The Journal of Physical Chemistry B*, Vol. 125, 2021, pp. 9601–9609, <https://doi.org/10.1021/acs.jpcc.1c03763>.
37. Sato, T., “Molecular Dynamics Investigation of Static and Dynamic Interfacial Properties in Ice-Polymer Premelting Layers,” *arXiv preprint arXiv:2504.19628*, 2025, <https://doi.org/10.1021/acs.jpcc.1c03763>.
38. Weng, L., “Molecular Dynamics at the Interface between Ice and Poly(vinyl alcohol) and Ice Recrystallization Inhibition,” *Langmuir*, Vol. 34, 2017, pp. 5116–5123, <https://doi.org/10.1021/acs.langmuir.7b03243>.

39. Naullage, P., “Molecular Recognition of Ice by Fully Flexible Molecules,” *The Journal of Physical Chemistry C*, Vol. 121, 2017, pp. 26949–26957, <https://doi.org/10.1021/acs.jpcc.7b10265>.
40. Bachtiger, F., “The Atomistic Details of the Ice Recrystallisation Inhibition Activity of PVA,” *Nature Communications*, Vol. 12, 2021, <https://doi.org/10.1038/s41467-021-21717-z>.
41. Su, C., “Ice Growth Inhibition by Poly(vinyl alcohol): Insights from Near-Infrared Spectroscopy and Molecular Dynamics Simulation,” *Journal of Molecular Liquids*, Vol. 402, 2024, pp. 124795, <https://doi.org/10.1016/j.molliq.2024.124795>.
42. Smith, J., “Hydrogen-Bonding Surfaces for Ice Mitigation,” *NASA Technical Reports Server*, 2014, <https://ntrs.nasa.gov/citations/20140011454>.
43. Hakimian, A., *Ice Adhesion: Mechanism, Measurement, and Mitigation*, chap. Metrology of Ice Adhesion, Wiley, 2020, pp. 217–237, <https://doi.org/10.1002/9781119640523.ch8>.
44. Laroche, A., *Ice Adhesion: Mechanism, Measurement, and Mitigation*, chap. Tensile and Shear Test Methods for Quantifying the Ice Adhesion Strength to a Surface, Wiley, 2020, pp. 238–284, <https://doi.org/10.1002/9781119640523.ch9>.
45. Ronneberg, S., *Ice Adhesion: Mechanism, Measurement, and Mitigation*, chap. Comparison of Icephobic Materials through Interlaboratory Studies, Wiley, 2020, pp. 285–324, <https://doi.org/10.1002/9781119640523.ch10>.
46. Rehfeld, N., “Round-Robin Study for Ice Adhesion Test,” *Aerospace*, Vol. 11, 2024, <https://doi.org/10.3390/aerospace11020106>.
47. Work, A., “A Critical Review of the Measurement of Ice Adhesion to Solid Substrates,” *Progress in Aerospace Sciences*, Vol. 98, 2018, pp. 1–26, <https://doi.org/10.1016/j.paerosci.2018.03.001>.
48. Work, A., “A Statistical Analysis of Impact Ice Adhesion Strength Data Acquired with a Modified Lap Joint Test,” AIAA, 2020, <https://doi.org/10.2514/6.2020-2801>.
49. Smith, J., “Impact Ice Adhesion Strength of Stainless Steel 304 as Determined on a Centrifuge Test Stand,” *Cold Regions Science and Technology*, 196, pp. 103492, <https://doi.org/10.1016/j.coldregions.2022.103492>.
50. Giuffre, C., “The Measurement of Shear Strain in Impact Ice Using a Modified Lap Joint Test and Digital Image Correlation,” *Proceedings of the AIAA AVIATION Forum*, AIAA, 2022, <https://doi.org/10.2514/6.2022-4071>.
51. Chen, R., “Impact Ice Microstructure Segmentation Using Transfer Learned Model,” *Proceedings of the SAE International Conference on Icing of Aircraft, Engines, and Structures*, SAE International, 2023, <https://doi.org/10.4271/2023-01-1410>.

52. Tenney, D., “Structural Framework for Flight: NASA’s role in Development of Advanced Composite Materials for Aircraft and Space Structures,” Contractor Report NAS/CR-2011-217076, NASA, 2011, <https://ntrs.nasa.gov/citations/20190002561>.
53. Ransom, J. B., “ARMD Workshop on Materials and Methods for Rapid Manufacturing for Commercial and Urban Aviation,” Technical Memorandum NAS/TM-2019-220428, NASA, 2019, <https://ntrs.nasa.gov/citations/20200000067>.
54. NASA, “The Material with a Need for Speed,” 2001.
55. Palmieri, F. L., “NASA CAS AERoBOND Project Summary,” White paper, NASA, 2020, <https://ntrs.nasa.gov/citations/20205001520>.
56. Zheng, J., “Vitrimers: Current Research Trends and their Emerging Applications,” *Materials Today*, Vol. 51, 2021, pp. 586–625, <https://doi.org/10.1016/j.mattod.2021.07.003>.
57. Lewis, B., “Glassy Dynamics of Epoxy-Amine Thermosets Containing Dynamic Aromatic Disulfide,” *Macromolecules*, Vol. 57, 2024, pp. 7112–7122, <https://doi.org/10.1021/acs.macromol.4c01012>.
58. Fu, Y., “A Hierarchical Energy Dissipated Structure Enabled Strong, Ultra-Tough, and Sustainable Adhesives,” *Advanced Functional Materials*, Vol. 34, 2024, pp. 2314561, <https://doi.org/10.1002/adfm.202314561>.
59. Westerman, C. R., “Sustainably Sourced Components to Generate High-Strength Adhesives,” *Nature*, Vol. 621, 2023, pp. 306–311, <https://doi.org/10.1038/s41586-023-06335-7>.
60. Zhu, Q., “Sustainable Snail-Inspired Bio-Based Adhesives with Ultra-High Adhesion,” *Advanced Functional Materials*, Vol. 34, 2024, pp. 2402734, <https://doi.org/10.1002/adfm.202402734>.
61. Raos, G., “Polymer Adhesion: Seeking New Solutions for an Old Problem,” *Macromolecules*, Vol. 54, 2021, pp. 10617–10644, <https://doi.org/10.1021/acs.macromol.1c01182>.
62. Hofman, A., “Bioinspired Underwater Adhesives by Using the Supramolecular Toolbox,” *Advanced Materials*, Vol. 30, 2018, pp. 1704640, <https://doi.org/10.1002/adma.201704640>.
63. Liu, J., “An Overview on the Adhesion Mechanisms of Typical Aquatic Organisms and the Applications of Biomimetic Adhesives in Aquatic Environments,” *International Journal of Molecular Sciences*, Vol. 25, 2024, pp. 7994, <https://doi.org/10.3390/ijms25147994>.
64. Wu, J., “Supramolecular Adhesives Inspired from Adhesive Proteins and Nucleic Acids: Molecular Design, Properties, and Applications,” *Soft Matter*, 2025, <https://doi.org/10.1039/D4SM01220H>.

65. Min, T., "Recent Advances in Barnacle-Inspired Biomaterials in the Field of Biomedical Research," *Materials*, Vol. 18, 2025, pp. 502, <https://doi.org/10.3390/ma18030502>.
66. So, C., "Sequence basis of Barnacle Cement Nanostructure is Defined by Proteins with Silk Homology," *Scientific Reports*, Vol. 6, 2016, pp. 36219, <https://doi.org/10.1038/srep36219>.
67. Trossmann, V., "Factors Influencing Properties of Spider Silk Coatings and Their Interactions within a Biological Environment," *Journal of Functional Biomaterials*, Vol. 14, 2023, pp. 434, <https://doi.org/10.3390/jfb14080434>.
68. Melrose, J., "High Performance Marine and Terrestrial Bioadhesives and the Biomedical Applications They Have Inspired," *Molecules*, Vol. 27, 2022, pp. 8982, <https://doi.org/10.3390/molecules27248982>.
69. Pawlicki, J., "The Effect of Molluscan Glue Proteins on Gel Mechanics," *Journal of Experimental Biology*, Vol. 207, 2004, pp. 1127–1135, <https://doi.org/10.1242/jeb.00859>.
70. Graham, L., "The Adhesive Skin Exudate of Notaden Bennetti Frogs (Anura: Limnodynastidae) has Similarities to the Prey Capture Glue of Euperipatoides sp. Velvet Worms (Onychophora: Peripatopsidae)," *Comparative Biochemistry and Physiology Part B: Biochemistry and Molecular Biology*, Vol. 165, 2013, pp. 250–259, <https://doi.org/10.1016/j.cbpb.2013.04.008>.
71. Wang, K., "Elastin Structure, Synthesis, Regulatory Mechanism and Relationship With Cardiovascular Diseases," *Frontiers in Cell and Developmental Biology*, Vol. 9, 2021, <https://doi.org/10.3389/fcell.2021.596702>.
72. Lin, C., "Comparison between Catechol- and Thiol-Based Adhesion Using Elastin-like Polypeptides," *ACS Applied Bio Materials*, Vol. 3, 2020, pp. 3894–3905, <https://doi.org/10.1021/acsabm.0c00431>.
73. Shi, J., "Strong Bioadhesives from Helical Polypeptides," *ACS Macro Letters*, Vol. 14, 2025, pp. 299–305, <https://doi.org/10.1021/acsmacrolett.5c00021>.
74. Liang, C., "Design of a Thermoresponsive, Scalable, and Robust Recombinant Protein-Based Bioadhesive by Combining Elastin-like Polypeptide with Barnacle Cement Protein," *ACS Biomaterials Science and Engineering*, Vol. 11, 2025, pp. 4116–4127, <https://doi.org/10.1021/acsbmaterials.5c00880>.
75. Sun, P., "Dopamine Containing Mussel Mimetic Polyurethane," *Acta Polymerica Sinica*, Vol. 8, 2009, pp. 803–808, <https://doi.org/10.3724/SP.J.1105.2009.00803>.
76. Matos-Perez, C., "Polymer Composition and Substrate Influences on the Adhesive Bonding of a Biomimetic, Cross-linking Polymer," *Journal of the American Chemical Society*, Vol. 134, 2012, pp. 9498–9505, <https://doi.org/10.1021/ja303369p>.

77. Schmidt, G., “Tunable Tannic Acid-Zein Adhesives for Bonding Different Substrates,” *Advanced Sustainable Systems*, Vol. 6, 2022, pp. 2100392, <https://doi.org/10.1002/adsu.202100392>.
78. Oude Vrielink, A., “Interaction of Ice Binding Proteins with Ice, Water and Ions,” *Biointerphases*, Vol. 11, 2016, <https://doi.org/10.1116/1.4939462>.
79. Gharib, G., “Antifreeze Proteins: A Tale of Evolution From Origin to Energy Applications,” *Frontiers in Bioengineering and Biotechnology*, Vol. 9, 2022, <https://doi.org/10.3389/fbioe.2021.770588>.
80. Meng, Y., “Preparation of Biological Antifreeze Protein-modified Emulsified Asphalt Coating and Research on its Anti-icing Performance,” *Construction and Building Materials*, Vol. 294, 2021, pp. 123473, <https://doi.org/10.1016/j.conbuildmat.2021.123473>.
81. Peng, C., “A Multilayer Photothermal Superhydrophobic Anti-Icing Coating Applied to Asphalt Pavement with Remarkable Wear Resistance,” *ACS Appl Mater Interfaces*, *ACS Applied Materials and Interfaces*, Vol. 16, 2024, pp. 35588–35603, <https://doi.org/10.1021/acsami.4c07193>.
82. Gao, Y., “Beetle and Mussel-Inspired Chimeric Protein for Fabricating Anti-Icing Coating,” *Colloids and Surfaces B: Biointerfaces*, Vol. 210, 2022, pp. 112252, <https://doi.org/10.1016/j.colsurfb.2021.112252>.
83. Kanganovich, M., “Spontaneous Formation of a Sustainable Antifreeze Coating by Peptide Self-Assembly,” *ACS Applied Materials and Interfaces*, Vol. 17, 2025, pp. 16256–16267, <https://doi.org/10.1021/acsami.4c22816>.
84. Yu, J., “Antifreeze Protein-Inspired Zwitterionic Graphene Oxide Nanosheets for a Photothermal Anti-icing Coating,” *Nano Letters*, Vol. 25, 2025, pp. 987–994, <https://doi.org/10.1021/acs.nanolett.4c04478>.
85. Zhong, J., “Multifunctionality in Nature: Structure-Function Relationships in Biological Materials,” *Biomimetics*, Vol. 8, 2023, pp. 284, <https://doi.org/10.3390/biomimetics8030284>.
86. Li, C., “Stimuli-Responsive Surfaces for Switchable Wettability and Adhesion,” *Journal of the Royal Society Interface*, Vol. 18, 2021, <https://doi.org/10.1098/rsif.2021.0162>.
87. Hudait, A., “Preordering of Water is not Needed for Ice Recognition by Hyperactive Antifreeze Proteins,” *Proceedings of the National Academy of Sciences*, Vol. 115, 2018, pp. 8266–8271, <https://doi.org/10.1073/pnas.1806996115>.
88. Eickhoff, L., “Contrasting Behavior of Antifreeze Proteins: Ice Growth Inhibitors and Ice Nucleation Promoters,” *The Journal of Physical Chemistry Letters*, Vol. 10, 2019, pp. 966–972, <https://doi.org/10.1021/acs.jpcclett.8b03719>.

89. Zhang, Y., “Fully Atomistic Molecular Dynamics Simulation of Ice Nucleation near an Antifreeze Protein,” *Journal of the American Chemical Society*, Vol. 147, 2025, pp. 4411–4418, <https://doi.org/10.1021/jacs.4c15210>.
90. Kozuch, D. J., “Combined Molecular Dynamics and Neural Network Method for Predicting Protein Antifreeze Activity,” *Proceedings of the National Academy of Sciences*, Vol. 115, 2018, pp. 13252–13257, <https://doi.org/10.1073/pnas.1814945115>.
91. Kozuch, D. J., “Genetic Algorithm Approach for the Optimization of Protein Antifreeze Activity using Molecular Simulations,” *Journal of Chemical Theory and Computation*, Vol. 16, 2020, pp. 7866–7873, <https://doi.org/10.1021/acs.jctc.0c00773>.
92. Kumar, A., “Disorder-order Interplay of a Barnacle Cement Protein Triggered by Interactions with Calcium and Carbonate Ions: A Molecular Dynamics Study,” *Chemistry of Materials*, Vol. 32, 2020, pp. 8845–8859, <https://doi.org/10.1021/acs.chemmater.0c02319>.
93. Yeh, I. C., “Molecular Dynamics Simulations of Adsorption of Catechol and Related Phenolic Compounds to Alumina Surfaces,” *The Journal of Physical Chemistry C*, Vol. 119, 2015, pp. 7721–7731, <https://doi.org/10.1021/jp512780s>.
94. Saiz-Poseu, J., “Self-assembly of a Catechol-based Macrocyclic at the Liquid-Solid Interface: Experiments and Molecular Dynamics Simulations,” *Physical Chemistry Chemical Physics*, Vol. 14, 2012, pp. 11937–11943, <https://doi.org/10.1039/C2CP41407D>.
95. Abramson, J., “Accurate Structure Prediction of Biomolecular Interactions with AlphaFold 3,” *Nature*, Vol. 630, 2024, pp. 493–500, <https://doi.org/10.1038/s41586-024-07487-w>.
96. Passaro, S., “Boltz-2: Towards Accurate and Efficient Binding Affinity Prediction,” *BioRxiv*, 2025, <https://doi.org/10.1101/2025.06.14.659707>.
97. Quijano-Rubio, A., “De Novo Design of Modular and Tunable Protein Biosensors,” *Nature*, Vol. 591, 2021, pp. 482–487, <https://doi.org/10.1038/s41586-021-03258-z>.
98. Watson, J. L., “De Novo Design of Protein Structure and Function with RF Diffusion,” *Nature*, Vol. 620, 2023, pp. 1089–1100, <https://doi.org/10.1038/s41586-023-06415-8>.