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# Reducing Vehicle Weight and Improving U.S. Energy Efficiency Using Integrated Computational Materials Engineering

WILLIAM J. JOOST[1,2]

1.—Vehicle Technologies Program, U.S. Department of Energy, 1000 Independence Ave., S.W., Washington, DC 20585, USA. 2.—e-mail: william.joost@ee.doe.gov

Transportation accounts for approximately 28% of U.S. energy consumption with the majority of transportation energy derived from petroleum sources. Many technologies such as vehicle electrification, advanced combustion, and advanced fuels can reduce transportation energy consumption by improving the efficiency of cars and trucks. Lightweight materials are another important technology that can improve passenger vehicle fuel efficiency by 6–8% for each 10% reduction in weight while also making electric and alternative vehicles more competitive. Despite the opportunities for improved efficiency, widespread deployment of lightweight materials for automotive structures is hampered by technology gaps most often associated with performance, manufacturability, and cost. In this report, the impact of reduced vehicle weight on energy efficiency is discussed with a particular emphasis on quantitative relationships determined by several researchers. The most promising lightweight materials systems are described along with a brief review of the most significant technical barriers to their implementation. For each material system, the development of accurate material models is critical to support simulation-intensive processing and structural design for vehicles; improved models also contribute to an integrated computational materials engineering (ICME) approach for addressing technical barriers and accelerating deployment. The value of computational techniques is described by considering recent ICME and computational materials science success stories with an emphasis on applying problem-specific methods.

## INTRODUCTION

There have been significant advances in the structural material technologies deployed in modern vehicles over the past decade; however, vehicle weight has continued to increase as a result of improvements in vehicle safety, emissions control, and creature comfort.[1] Safety, emissions control, and comfort are all important features, so the challenge is to maintain (or improve) performance in these categories while reducing mass. While improved materials are necessary to achieve weight savings without sacrificing performance, the property, manufacturability, and cost requirements for automotive structures are often not met by the existing set of advanced lightweight materials and further development is needed. The classic development to deployment process for new materials requires many years or even decades to complete. Even when new materials are deployed, it is often difficult to optimize their use in the context of multiple vehicle performance variables such as weight, cost, crash behavior, surface finish, etc. The design process for vehicle structures and manufacturing processes relies heavily on simulation, necessitating accurate models for the behavior of lightweight materials. Such models also contribute to an integrated computational materials engineering (ICME)[2] approach and to the vision of the Materials Genome Initiative;[3] ICME is a promising technique for reducing the time required for development and deployment of new materials while also providing opportunities for optimization against a variety of important response variables without the need for large experimental matrices and iterative testing. Ongoing research and development work provides examples of computational techniques and ICME applied towards alloy development, process development, and integrated materials/structural design—all critical for achieving vehicle weight

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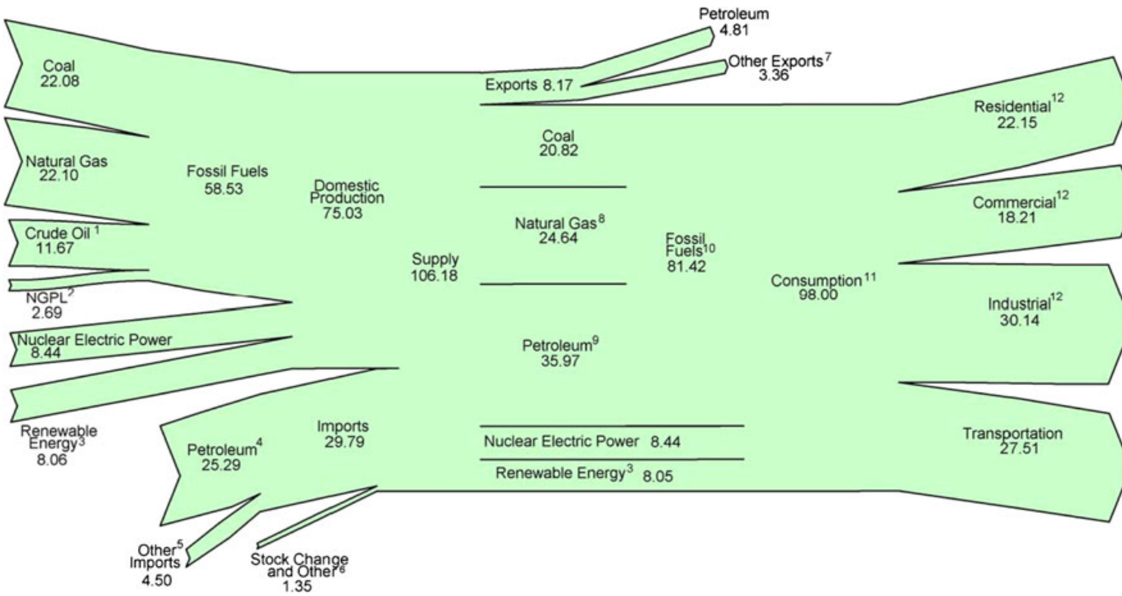


Fig. 1. Total U.S. energy flow, 2010 (QBtu), from Ref. 4.

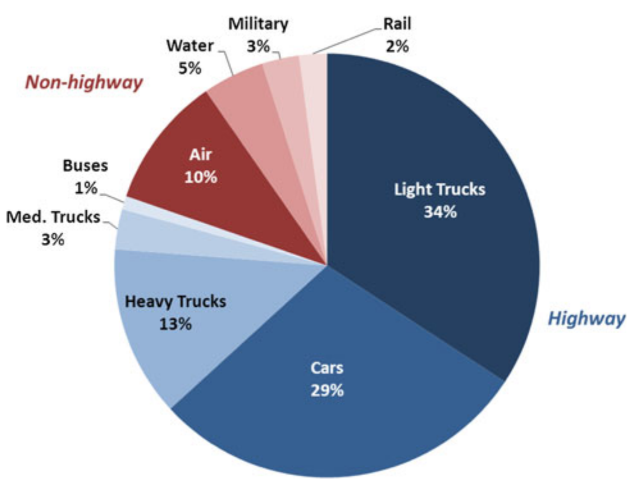


Fig. 2. U.S. transportation energy, relative consumption by mode, 2009. Data from Ref. 4.

reduction and the attending improvement in U.S. transportation energy efficiency.

In this report, the relationship between vehicle weight and U.S. transportation energy is discussed starting with a high-level view of U.S. energy then working down towards an understanding of how mass affects efficiency in passenger and commercial vehicles. A review of the most promising lightweight materials and significant technology gaps outlines the need for research and development work across a wide range of materials, vehicle applications, and enabling technologies. Finally, a review of several recent computational materials activities provides insight to how computation and ICME projects tailored to the required outcomes provide the best opportunity for impact in vehicle weight reduction.

## THE U.S. ENERGY LANDSCAPE

Energy is a diverse, complicated topic, and the relationship between vehicle weight and energy consumption can be more easily understood by first considering the overall U.S. energy landscape. The consumers of energy in the United States can be divided into four sectors: residential (our homes), commercial (such as office buildings and shopping malls), industrial (such as manufacturing), and transportation (passenger and commercial vehicles, rail, air, and marine). Figure 1 provides the total U.S. energy flow during 2010 in quadrillion British thermal units (QBtu), or "quads." Transportation accounted for approximately 28% of the total energy consumed in the U.S. in 2010. However, the different sectors derive energy from different sources, and transportation energy is supplied mostly from petroleum. In fact, the transportation sector consumed about 13.5 million barrels per day (Mbpd) of oil in 2010, 71% of the total petroleum consumed across all sectors.[4] Reducing energy consumption in the transportation sector can, therefore, significantly reduce total U.S. energy consumption while having a disproportionate impact on U.S. petroleum consumption. A variety of technical developments can support reduced transportation energy consumption including combustion efficiency improvements, advanced fuels and lubricant development, effective vehicle electrification, and reduction of vehicle weight.

Within the transportation sector, energy consumption is divided into highway modes, which include commercial and passenger vehicles, and nonhighway modes, which include air, rail, and marine. Figure 2 shows the relative energy consumption by mode, demonstrating that passenger and commercial vehicles (highway modes) account for the majority of transportation energy consumption, more than 5.3 Mbpd of petroleum.[4] Transportation energy consumption by passenger and commercial vehicles is therefore a significant component of the total U.S. energy landscape, and understanding the quantitative relationship between weight and efficiency is necessary to better appreciate the importance of mass reduction.

## THE IMPACTS OF VEHICLE WEIGHT REDUCTION ON ENERGY EFFICIENCY

Reducing vehicle weight affects transportation energy consumption by improving efficiency. More than 85% of the energy in fuel is lost to thermal and mechanical inefficiency in the drivetrain,[5] while the remaining 12–15% is used to overcome the tractive forces that resist forward motion.[6] Of these tractive forces, vehicle weight most significantly affects inertial (acceleration) and rolling resistance forces. Aerodynamic forces are not directly related to mass but can be correlated in some cases. While the specific relationships between mass and inertial and friction forces are well understood, calculating the exact impact of vehicle weight reduction on overall fleet energy efficiency is complicated by factors such as fleet mix, mass decompounding, and vehicle design decisions. Several studies have explored the relationship between mass and fuel consumption using empirical techniques. A linear regression analysis of curb weight versus carbon dioxide ($CO_2$) emissions (a measure of efficiency that is correlated with fuel consumption) for the model year 2008 vehicle fleet suggests that a 10% reduction in vehicle weight is associated with an 8% reduction of $CO_2$ emissions.[7] A model that combines curb weight and fuel consumption data with a technique for normalizing vehicle performance indicates that a 10% reduction in vehicle weight yields a 5.6% reduction in fuel consumption for cars and a 6.3% reduction in fuel consumption for light trucks.[6] Other studies have used more complicated models. A detailed model of vehicle performance as a function of mass across several driving cycles shows a 6.8% improvement in fuel economy for a 10% reduction in vehicle weight when the engine is "resized" to maintain the performance characteristics of the original vehicle;[8] simulation using a different detailed modeling technique indicates that a 10% reduction in weight provides a 6.9% reduction in fuel consumption for cars and a 7.6% reduction in fuel consumption for light trucks.[9] Modeling work at the National Renewable Energy Laboratory (NREL) also uses a detailed model to understand vehicle efficiency and predicts a 6.9% improvement in fuel economy for a 10% reduction in weight when the engine is resized. Despite the varied approaches summarized here, the results are quite similar. In general, a 10% reduction in vehicle weight provides a 6–8% improvement in fuel economy when vehicle performance characteristics are maintained.*

Reducing vehicle weight can also have a less obvious effect on transportation energy consumption by making electric vehicles (EVs), alternative fuel vehicles (AFVs), and highly efficient conventional vehicles more competitive. While EVs have the potential to improve transportation energy efficiency, consumer concerns about cost, electric range, and performance limit their impact. A 10% weight reduction for an electric vehicle can improve electric range by 13.7%[10] while NREL modeling results show a 5.1% improvement in fuel economy for a 10% weight reduction in a hybrid electric vehicle. By improving electric range, weight reduction creates a larger design window for vehicle manufacturers, which can, in turn, affect consumer acceptance. For example, reducing the weight of an EV allows the vehicle designer to improve electric range (while maintaining battery size/cost), reduce battery size/cost (while maintaining electric range), or find the optimal balance to meet consumer expectations in the specific vehicle segment. A recent study conducted by General Motors provides an example of optimizing EV weight and battery size, finding that total vehicle cost can be reduced by lighweighting.[11] Similarly, weight reduction increases the cost/performance optimization window for AFV and highly efficient conventional vehicles, such as by maintaining low acceleration times while reducing engine size.

Weight reduction can also improve the efficiency of heavy duty vehicles, such as the "semis" that move a significant amounts of cargo around the United States. The nature of heavy duty trucking offers a different focus for the impact of weight reduction. While the fuel efficiency of heavy-duty vehicles improves with reduced weight, a more practical use of weight reduction is for improved freight efficiency (e.g., ton-miles per gallon). For example, a typical class 8 tractor weighs approximately 16,000 pounds while the empty trailer weighs approximately 13,000 pounds. A fully loaded truck has a maximum allowable weight of 80,000 pounds, meaning that approximately 51,000 pounds of cargo can be loaded representing 64% of the total weight. Because of this weight distribution, reducing the structural weight of the tractor and trailer by 50% only reduces the total loaded weight by 23%. Instead of reducing the total weight, a more efficient option may be to load the truck back to 80,000 pounds with additional cargo, increasing the total delivered tonnage for the same fuel use.

*It is important to note that a 7% reduction in fuel consumption (gallons per mile) is not the same as a 7% increase in fuel economy (miles per gallon). For changes on the order of 10%, the improvements are similar and the terms can be used somewhat interchangeably.

## MATERIALS ENGINEERING CHALLENGES IN LIGHTWEIGHTING

There is an immense variety of materials available to support vehicle weight reduction; however, five categories show the most promise: advanced high strength steels (AHSS), aluminum alloys, magnesium alloys, fiber reinforced polymer composites (including carbon and glass fibers), and advanced polymers (without fiber reinforcement). Other materials such as metal matrix composites, titanium alloys, nickel alloys, and advanced glazings (glass, polycarbonate, etc.) are also considered, although limited applications and significant barriers may reduce their weight reduction potential. Deployment of any new material into high-volume automotive production is limited by performance, manufacturability, and cost. As vehicle design and testing is now highly reliant on computer simulation, accurate models of material behavior during manufacturing and vehicle operation are also necessary; further, integration of these models with materials data, experimental results, and performance and manufacturing simulation tools constitute the ICME approach with its attending benefits. There are significant technical hurdles to improved performance, manufacturability, cost, and modeling for each of the five main material systems, for example:

*Advanced high-strength steels*—No identified microstructures for meeting both strength and ductility requirements of third-generation AHSS; susceptibility to local failure during forming and crash; difficulty incorporating significant hardening/softening behavior associated with forming and joining into processing and design models.
*Aluminum alloys*—Limited formability of automotive grades at room temperature; relatively high cost of sheet material; difficulty casting complex, high-strength parts; insufficient strength and/or stiffness for certain structural applications.
*Magnesium alloys*—Very low formability of sheet alloys at room temperature; challenge cost-effectively preventing galvanic corrosion; insufficient strength, ductility, and stiffness for certain structural applications; difficulty incorporating unique deformation behavior into processing and design models.
*Fiber-reinforced polymer composites*—High cost of carbon fiber; limited weight reduction potential of glass fiber; long cycle times for many process; difficulty incorporating structure at many length scales into processing and design models.
*Advanced polymers*—Low cure rates associated with ease of mold filling increases cycle times; petroleum-based precursors are dependent upon the price of oil while nonpetroleum precursors are not yet mature; susceptible to deterioration during high-temperature processing such as in automotive paint ovens.

A further complication to significant vehicle weight reduction is the need for multimaterial solutions. Each of the materials listed above (and perhaps any material) is optimal for certain applications but unlikely to provide an ideal solution for all components and functions in a vehicle. Material substitution at the component level can reduce weight through the application of materials with improved specific properties (i.e., properties per unit density) or by consolidation of parts and functions. Examples of component level material substitution are shown in Fig. 3; the AHSS rear chassis structure[12] and magnesium engine cradle[13] both reduce considerable weight while maintaining the specific packaging and performance requirements of the original steel components. Material substitution can also occur at the system level, such as in the examples shown in Fig. 4. In both of these examples, the global packaging and functional requirements are maintained but the requirements for each component are modified to yield a more optimized design. While neither is an example of a total-vehicle holistic lightweight design, both suggest impressive weight savings while notably requiring the use of various material types. In the case of the magnesium intensive vehicle front end (Fig. 4a) several aluminum components were introduced to provide adequate performance.[14] The European Union Super Light Car (EU SLC) is about 50% aluminum by weight but also includes significant use of magnesium, steel, and composites.[15] The requirement for multimaterial solutions introduces an additional layer of technology challenges associated with multimaterial joining, corrosion prevention, design tools, and performance predictions.

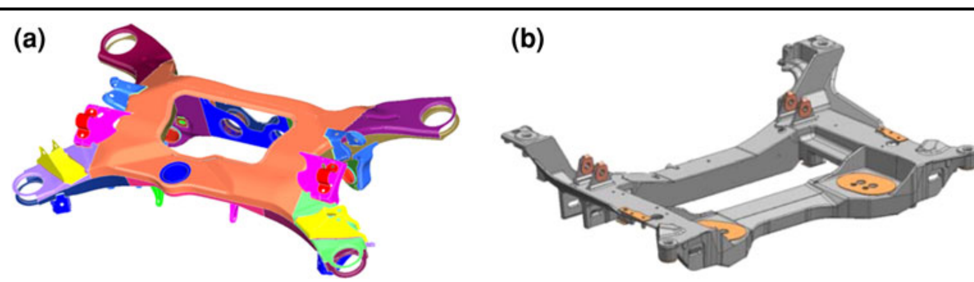


Fig. 3. (a) AHSS rear chassis structure with 28% weight reduction versus conventional steel baseline, from Ref. 12. (b) Magnesium engine cradle with 35% weight reduction versus conventional aluminum baseline, from Ref. 13.

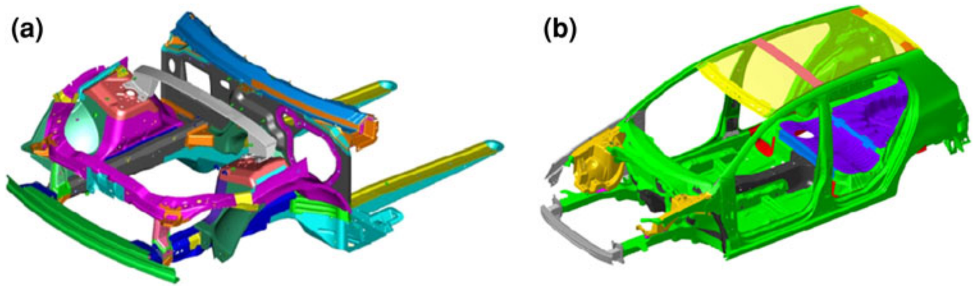


Fig. 4. (a) U.S. Automotive Materials Partnership (USAMP)/Department of Energy magnesium intensive vehicle front end with 45% weight reduction versus baseline (baseline shown), from Ref. 14. (b) European Union Super Light Car with 35% weight reduction versus baseline, from Refs. 15 and 16.

Overcoming these technical hurdles requires considerable materials science effort and new discovery with the outcomes constrained by the cost and performance requirements of automotive manufacturing. Classically, the discovery to deployment process for materials solutions with this combination of significant barriers and rigid constraints would require decades. However, near term transportation energy reduction is necessary, and so novel methods for rapidly developing and deploying new materials are required. One promising path to accelerating the development to deployment cycle is through the use of ICME, defined as "the integration of materials information, captured in computational tools, with engineering performance analysis and manufacturing-process simulation."[2] ICME is an approach that can reduce research and development (R&D) time by replacing experimental iteration, helping to identify unique opportunities in the processing-structure-properties relationships in materials, and providing valuable insight into the fundamental mechanisms that drive specific behavior. ICME continues to grow as a field, with increased emphasis after the 2011 announcement of the Materials Genome Initiative, an interagency effort that supports development of the material models, the implementation framework, and the data analytics tools necessary to solve industrially relevant materials engineering problems using an ICME approach.[3] While considerable momentum has accumulated, realizing the potential impact of ICME techniques on automotive lightweighting problems will require further development of the technology, the infrastructure, and the community.

## INTEGRATED COMPUTATIONAL MATERIALS ENGINEERING FOR VEHICLE WEIGHT REDUCTION

Overcoming the technical gaps that prevent the widespread adoption of lightweight automotive materials will require the full toolset of the materials engineering community, including computational techniques. Computational materials science and ICME is receiving increased attention as an important method in materials science due in part to a growing list of success stories. Within the automotive industry, the Ford Virtual Aluminum Castings[17] and General Motors Virtual Cast Component Development[18] projects have both demonstrated the potential of an ICME approach in improving powertrain castings. Computational materials techniques have also shown initial success in predicting the behavior of important structural automotive materials. Research in wrought aluminum alloys has yielded promising results from first-principles predictions of solute strengthening[19] and multiscale modeling of warm formability[20]; these techniques support overcoming two of the significant technology barriers to increased aluminum content in vehicles, namely insufficient strength and limited formability in aluminum alloys. Similar work has helped to address significant technology barriers within magnesium alloys systems, such as overcoming limited thermodynamic and kinetic data[21] and efficiently exploring the strengthening potency of various alloying additions.[22] These projects demonstrate that ICME and computational materials science can be effective approaches for improving product performance and addressing the barriers to deployment of materials that reduce vehicle weight.

The exact computational or ICME approach that is appropriate for a given automotive lightweighting problem will vary considerably with the requirements for the solution. Some engineering problems require detailed, quantitative results while others may only require qualitative guidance for research. One aspect of "detail" is the balance between scalability and specificity in modeling and integration techniques. A highly scalable method would support a wide array of materials and data types with general modeling techniques across many length scales. A highly specific approach supports the development of models particularly suited to a given problem and material set with correspondingly specific data structures. While scalable solutions may be more applicable in subsequent research, specific solutions may be easier to develop and implement. A correctly posed foundational engineering problem (FEP)[2] can help define the correct balance of scalability and specificity. A second aspect of "detail" is the incorporation of phenomena from various length scales. A passenger vehicle is comprised of roughly $10^{28}$ atoms; hence, explicitly simulating atomic (or subatomic) behavior for an entire car is computationally intractable. However, the macroproperties of materials are derived from structure and behavior at the atomic scales, nanoscales, and mesoscales; therefore, feasible methods for integrating results between models at angstrom and meter length scales are needed. Here again, the requirements of the FEP guides the application of models from necessary scales. A third aspect of an ICME approach is the integration of experimental data for model input, model validation, and insight. Recent automotive lightweight materials R&D using computational materials science and ICME demonstrates the usefulness of an appropriately detailed approach and the importance of integrated experimental and computational techniques.

A very specific FEP may be addressed by suitably specific models and reliance on significant experimental data. For example, Kahn et al. report a study assessing the durability of Al 2024 sheet components for a particular aircraft fuselage stringer assembly.[23] The desired output from this study is specific to an alloy, application, and loading condition, and therefore, significant experimental data were collected and used to determine the model type (ductile–brittle damage model in this case), provide model parameters, and validate model results. While not widely applicable across many industries and material types, the results from this work are useful in improving the design of aircraft structures produced in Al 2024 to increase durability, an important performance measure. The focused FEP yielded a similarly focused ICME approach and considerable influence of experimental data on modeling results.

A slightly more general example FEP is reported by Saeed-Akbari et al.[24] Here, the focus is on predicting deformation mode and hardening behavior in twinning-induced plasticity (TWIP) steels as a function of alloy chemistry and the resulting change in stacking fault energy (SFE). While focused on a specific class of materials (TWIP sheet steels), this more general FEP considers a range of alloys. A combination of first principles and thermodynamic modeling with mechanical and thermodynamic test data is used to provide guidance for alloy design in higher performance TWIP steel. A significant barrier to the introduction of TWIP steels in automotive manufacturing is the high cost, largely due to the cost of alloying ingredients. These models provide insight to the effect of chemistry on deformation behavior, potentially revealing a path towards lower cost TWIP steels. This more general FEP requires an approach utilizing models across more scales and incorporating more general thermodynamic data from experiment.

A highly scalable and very interesting study is reported by Leyson et al.[19] These researchers present a parameter-free model, based on first-principles calculations of interactions between solute atoms and edge dislocations that is able to predict the tensile yield stress of aluminum alloyed with Mg, Cr, Cu, and Mg–Si. This approach requires no input from experimental data and is generally applicable to studying solute strengthening in other alloy systems. However, experimental results still play a very important role in validating the model results; in this case, experimental data indicate that the model underpredicts tensile strength unless impurity concentrations of Fe are considered—an important result when using such a model for guidance in developing new alloys. While this is a very general computational approach (in the sense that it could be applied to many solute additions in many alloy systems for a variety of applications), the computational modeling occurs only at low length scales, feeding analytical models at somewhat higher length scales. This example demonstrates a “general” FEP such as this does not necessarily correlate to the application of models across a wider range of length scales. Rather, the objectives of the FEP dictate the modeling requirements that in turn determine the types of models, the appropriate length scales, and the required integration of experimental data.

These examples suggest that a universal method for determining the scalability, the incorporation of specific length scales, and the required experimental data does not exist. Rather, the characteristics of the desired solution for the FEP provide guidance on the approach. These examples also demonstrate how a properly focused computational and ICME approach can provide insight and thereby support accelerated deployment of materials for automotive lightweighting. Continued development of the materials models and integration techniques coupled with a growing list of success stories such as these will help to improve the usefulness of ICME and its impact on U.S. energy consumption.

## CONCLUSION

Reducing vehicle weight can help decrease U.S. energy and petroleum consumption by increasing efficiency in conventional vehicles and improving competitiveness in electric vehicles, AFVs, and highly efficient conventional vehicles. Despite the significant potential of vehicle weight reduction, widespread automotive deployment of advanced high-strength steels, aluminum alloys, magnesium alloys, fiber reinforced composites, and advanced polymers is limited by a variety of technical challenges that require continued research and development. Optimal lightweight designs typically require the use of multimaterial structures, presenting additional technology gaps associated with joining, corrosion protection, and design. Rapidly addressing these challenges requires supplementing classical materials R&D techniques with computational materials science and ICME. Recent success in applying ICME techniques towards the development of automotive materials highlights the potential of this approach; however, continued improvement of the modeling, data, experimental, and integration techniques is needed. With particular regard towards specificity/scalability, multiscale modeling, and integration of experimental data, recently published research demonstrates that the FEP requirements help to guide the detailed requirements of the computational approach and yield the most useful results. As ICME continues to mature, both as a field and a technique, faster material development and deployment will help to more rapidly introduce lightweight materials, reduce vehicle weight, and improve U.S. energy efficiency.

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