INTEGRATED COMPUTATIONAL MATERIALS ENGINEERING
ACCELERATING MATERIALS DEVELOPMENT AND MANUFACTURING
What Is ICME?
Integrated Computational Materials Engineering (ICME) combines bedrock computational physics and informatics with systematic experiments and advanced manufacturing to reduce the cost, risk, and cycle time for new product development. It merges a top-down approach using state-of-the-art informatics tools to mine an extensive database on materials, product properties, and manufacturing process performance with bottom-up multiscale modeling based on first principles.

At Lockheed Martin, ICME is enabling Lockheed Martin engineers to concurrently design materials, components, and flexible manufacturing processes to reduce technology insertion risks for major programs. Potential savings from ICME will come at every step of the design and manufacturing process:

- Conceptual design
- Material selection and qualification
- Component design trades
- Process selection, development and optimization
- Device design and integration
- Process verification
- Assembly and testing
- Part certification
- Low rate initial production
- Repair, maintenance, and sustainment.

ICME has already benefited several programs at Lockheed Martin.

Materials Design
During the development of the APEX family of multiscale reinforced nanocomposites, the ICME team modeled the unique behavior of the nano- and microscale constituents that make up these materials. Through a multiscale modeling approach combining computational fluid dynamics, orthotropic laminate analysis, and continuum mechanics, changes in APEX constituents and thermal process conditions, can be translated into predictions of part performance at the design stage.

Chemical Sensors
Lockheed Martin’s development of chemical sensors is also benefitting from its expertise in ICME. To help design an electronic nose sensory array for civil and homeland security applications, the ICME team is modeling the interactions between carbon nanotubes and DNA at the molecular level. The resulting model provides the means to understand how changes in DNA structure influence the sensor’s ability to detect specific volatile organic chemicals and provides a means of optimizing the sensitivity and specificity of the sensor arrays during the design phase.

IR Sensing Platforms
ICME has made a significant contribution to the design of new electronic and energy platforms. Much of this work involves the development of new semiconductor materials designed to interface with silicon with minimal lattice mismatch. This work on integrated nanoelectronic multi-scale modeling of bandgap semiconductors has enabled Lockheed Martin engineers to design:

- Lower-cost integrated circuits for large format infrared focal plane arrays
- Strain Layer Superlattice semiconductor alloys with tailored infrared cutoff wavelengths and designed layer thicknesses for optimized absorption.

New Tools for Solving Problems with ICME
Lockheed Martin’s ICME efforts go beyond modeling activities. Lockheed Martin engineers are developing a suite of informatics tools and rapid characterization tools that will speed the calibration of empirical models that is needed to fill gaps in our theoretical understanding. Working with colleagues at the Air Force Research Laboratory, the ICME team is integrating this suite of tools into a high-throughput carbon nanotube materials discovery platform in order optimize the growth conditions for single-walled carbon nanotubes with specific electronic configurations. This work aims to enable device designers to tailor the bandgap of electro-optical devices such as infrared sensors.

The ICME team is also creating a new open and interoperable device modeling and design tool. The ultimate payoff will be the ability to design products from the top down and enable the digital factory that will provide flexible materials and manufacturing solutions—and a 3- to 9-fold return on investment from such ICME efforts.

Lockheed Martin ICME aims to move the field of materials science from one that designs products around materials to one that tailors materials to fit a specific use, and by doing so, reduce the costs of failure and redesign in the production of high-performance components for defense, aerospace, automotive, and other commercial applications.