

# Better Graphene-Epoxy Based Composite Materials with HPC

## Organizations

**Nanografi** is a manufacturer and supplier of advanced nanomaterials with one of Europe's largest graphene production plants.

**Alti Dynamics** is an SME focusing on advanced aerospace nanomaterial technologies.

**Middle East Technical University (METU)** is a Turkish public university that provides HPC expertise.

**TUBITAK ULAKBIM** is a Turkish national centre providing HPC and data storage to academia and industry.



End User



Technology Expert



HPC Expert



HPC Center



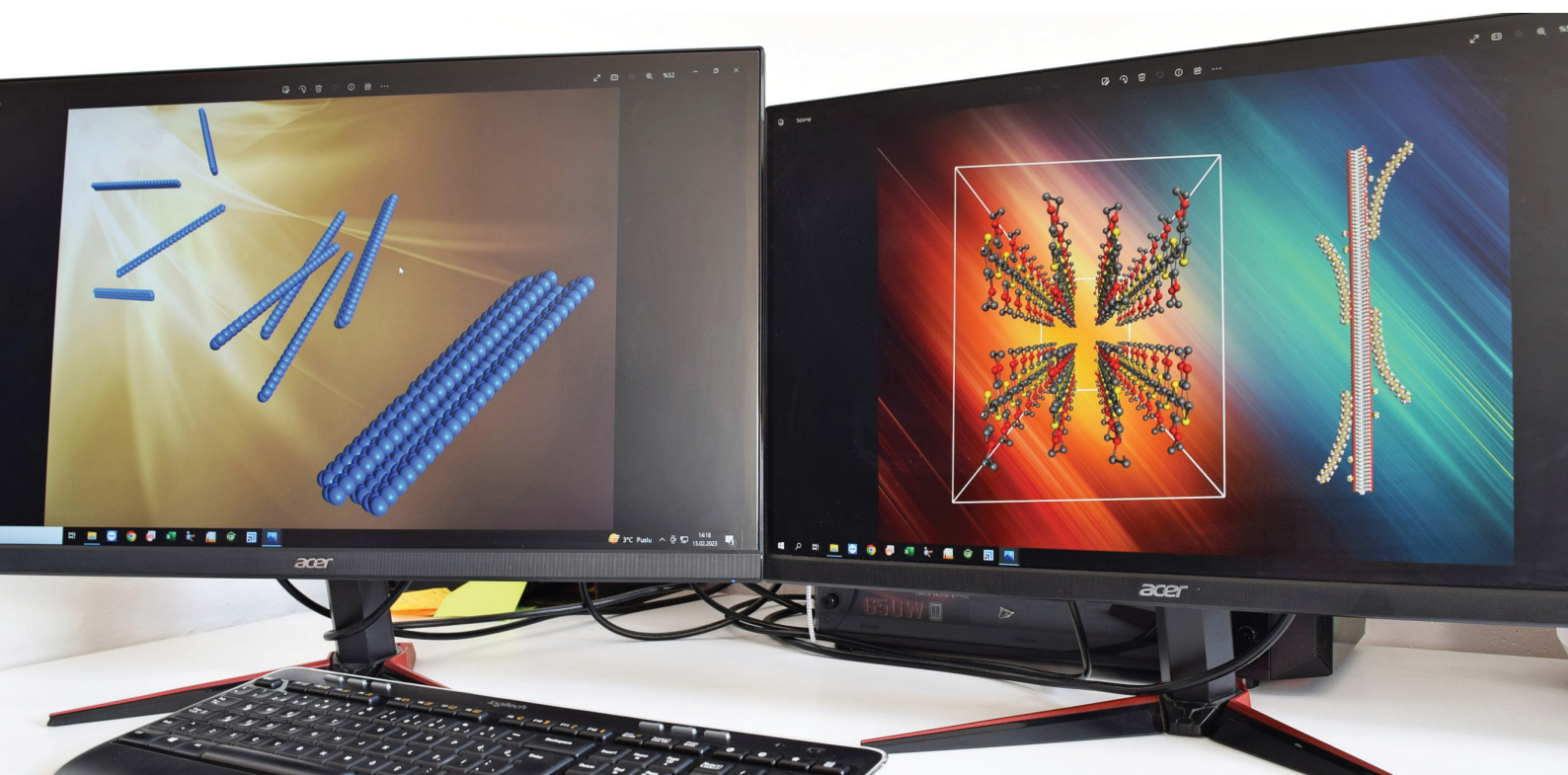
TUBITAK and METU are part of the Turkish NCC.

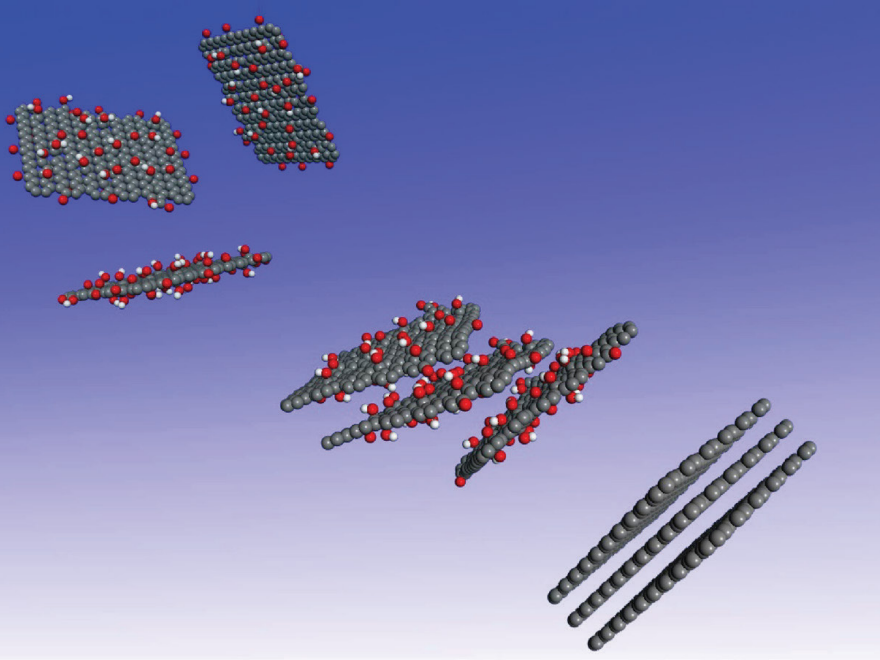


## The Challenge

Composite materials are composed of a base material, e.g., a polymer resin like epoxy (the matrix), and one or more additives giving it enhanced or special mechanical, thermal, or electrical properties.

Nanografi sells more than 1,000 advanced materials with nano- and micron-sized additives and one of the most popular products are nano-sized graphene and graphene oxide (GO)-enhanced polymer composites that are highly attractive as advanced materials in the aerospace industry due to their superior properties. These materials perform better in comparison to conventional epoxy-graphite composites with micro-sized large graphene aggregates. Alti Dynamics is a business partner of Nanografi specialising in the search for additives resulting in composites with enhanced properties and applications. Their current process is based on a "synthesize-test-improve" cycle with a lot of human resources spent in the trial-and-error stages to develop the composite with the best physical and mechanical properties. However, since many parameters influence these properties, such as the type of epoxy polymer, the dispersion of graphene layers, and pre-treatment conditions, these experiments are both costly and time-consuming. Moreover, homogeneous dispersion and strong adhesion of GO sheets to epoxy resin are crucial to enhance the properties of materials, yet obtaining highly dispersed graphene sheets and their enhanced interaction with the epoxy matrix is a challenge which is hard to meet solely through experiments. Therefore, Alti Dynamics was searching for ways to reduce both the related costs and the duration for obtaining patentable, optimised recipes for nano-composite production.





Industry Sector  
**Manufacturing**

Technology used:  
**HPC,**  
**MD Simulations,**  
**Monte Carlo Simulations**

## The Solution

The types and number of functional groups on GO, the mass percentage of GO in the resin matrix, and the structure of the epoxy resin were optimized with HPC simulations. The materials were manufactured, tested for material properties and simultaneously modelled by the HPC experts. With classical molecular dynamics simulations, which due to the size of the systems and level of interaction required HPC, strong candidates for the actual synthesis stage were identified.

## The Impact

Thanks to this experiment, Alti Dynamics is now using the results of the HPC-based simulations to obtain high-quality epoxy-graphene nanocomposite materials for various advanced aerospace applications, reducing development time by up to 15% and costs by up to 20% while increasing their competitiveness. The HPC results provided insights that led to optimised parameters for large-scale production and commercialisation of epoxy/GO nanocomposites with improved properties in less time and with higher accuracy. By moving to a simulation-based workflow, the companies expect to reduce testing material waste by 75% (approximately €260,000 savings per year) and raw material consumption by 40% (approximately €315,000 savings per year). The new capabilities of the HPC-based workflow will provide Alti Dynamics with a competitive advantage and a corresponding increase in revenue, which is expected to add €750,000 over the next 3-4 years.

Nanografi will be able to sell significantly more raw graphene products to customers, especially automotive and aerospace companies, and their suppliers, through the optimisation provided by Alti Dynamics' performance testing studies in collaboration with HPC simulations, which is a profitable advancement for both companies. Following the commercialisation activities of the industrial partners, graphene will gain a stronger foothold in the composites market as a mechanical performance-enhancing and weight-reducing additive that has highly desired properties for aerospace material applications.

## Benefits

- Alti Dynamics expects to save over €260,000 per year because fewer tests are necessary.
- Alti Dynamics expects an increase in revenue up to €750,000 during the next 3-4 years.
- Within 3 years, Nanografi expects to increase sales of graphene-related products by a factor of 10.