NCC success stories - Collaboration with industrial (end) users

1. Title

Improving the Efficiency of the Graphene-Enhanced Polymer Composite Production via Classical Molecular Dynamics

2. NCC presenting the success story

The leader of the NCC is TUBITAK-TRUBA, who is one of the two large HPC centers of Turkey. In addition to TRUBA, two academic partners Middle East Technical University (METU) and Sabanci University (SU) act as third parties. While METU is a public university based in Ankara, SU is a privately-funded university in Istanbul. Our competencies include High Performance Computing (HPC), High Performance Data Analytics (HPDA), Artificial Intelligence (AI), CUDA, Materials Science, Computational Fluid Dynamics (CFD) and several other fields. The particular third-party presenting this success story is the Middle East Technical University.

3. Industrial organisations Involved:

This success story is a result of a case study conducted by METU in collaboration with an SME (Nanografi) located in METU's Technopark. METU is a publicly-funded university with approximately 30000 students. It is considered both a teaching and a research university, recognized as such by the government. Founded in 2011, Nanografi (https://nanografi.com/) is a company that specializes in the production of nanomaterials including graphene-polymer composites, CVD-grown graphene, graphene oxide and fullerenes. Nanografi has a strong R&D department and has references from large companies such as Bosch, Intel and Xerox.

4. Technical/scientific Challenge:

One of the most popular products that Nanografi specializes in is graphene- and graphene oxide-enhanced polymer composites. Their protocol is based on a "synthesize-test-improve" with a lot of the human resources spent in the trial-and-error stages to develop the composite with the best mechanical properties. Since there are a large number of parameters that potentially go into this problem such as the type of the polymer, the sheet number of graphene, and pretreatment conditions, these experiments are both costly and time-consuming. The company would like to reduce the cost and duration of these experiments by means of pre-screening the parameter space via materials simulations. Our academic team from METU (Dr. Erol Yildirim and Dr. Hande Toffoli) in collaboration with our TRUBA specialist (Dr. Sevil Sarıkurt Malcıoğlu) have helped implement an alternative computational route for Nanografi to first model the composites using classical molecular dynamics (MD) to identify strong candidates before the actual synthesis stage.

5. Solution:

Our collaboration provided the following solutions:

- A company employee was trained and learned how to use HPC resources on the TRUBA computers. She also learned how to use the open-source code LAMMPS (https://www.lammps.org/) for conducting the calculations.
- Our academic expert, Dr. Erol Yıldırım set up a protocol for preparing and running different composites and trained the company employee on how to use this.
- The company had no prior experience in using HPC resources. For the first time in their history, they were introduced to these services.

6. Business impact:

The business impact for this collaboration is not expected to be immediate but instead rather long-term, following a gradual transition period. At the moment, the experimental protocol utilized by Nanografi is arduous and time-consuming. There is a vast parameter space related to the synthesis stage to be tried. Our team has proposed an alternative mechanism where the initial elimination of the composites to be synthesized is to be simulated using classical molecular dynamics. The results of the simulations will then be analyzed and strong composite candidates will be identified. The parameters that can be implemented in the calculations are the type of the polymer matrix, linker type, chain length, properties of the graphene-based enhancement material, and effects of temperature. The synthesis will then process within the much-reduced domain of these candidates. This will, in the long run, benefit the company by means of reducing both human resource needs and synthesis costs.

In addition, with this collaboration, the company was introduced, for the first time, to HPC services. Hopefully, this collaboration will motivate investment in HPC-literate personnel and their training in the long run.

Finally, our academic team, our TRUBA expert, and Nanografi (along with an end-user company) have submitted a proposal to the FF4EuroHPC call. We were able to work efficiently and in harmony. The areas of expertise of the various team members complemented one another rather nicely. This case study can therefore be seen as the beginning of a lifelong collaboration, which will surely benefit all parties involved.

7. Benefits:

This collaboration was mutually very beneficial for both parties.

<u>METU/TRUBA</u>

- has now gained access to R&D input from an industrial partner with no prior experience with HPC or infrastructure.
- could not have formed this sort of a partnership through which they were able to participate in the FF4EuroHPC call.

<u>Nanografi</u>

- were introduced to computational materials science and HPC services for the first time,

- were able to tap into computational work as an alternative or support mechanism to the traditional and rather time-consuming experimental methods,
- could not have formed this sort of a partnership through which they were able to participate in the FF4EuroHPC call.

Success story # Highlights:

- Keywords: *Polymer matrix composites, graphene materials, manufacturing, materials science, raw materials*
- Industry sector: *Aeronautics, Chemicals, Manufacturing & Engineering, Material sciences*
- Technology: *HPC*

Images:

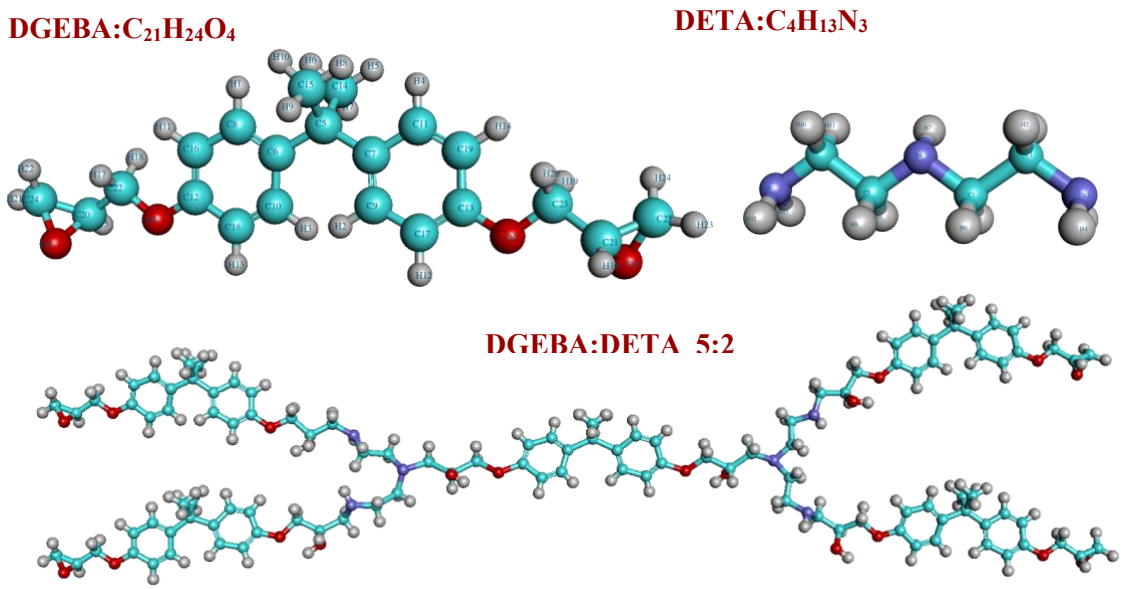

Figure 1: Molecular structure of DGEBA, DETA, and representative crosslinked epoxy chain.

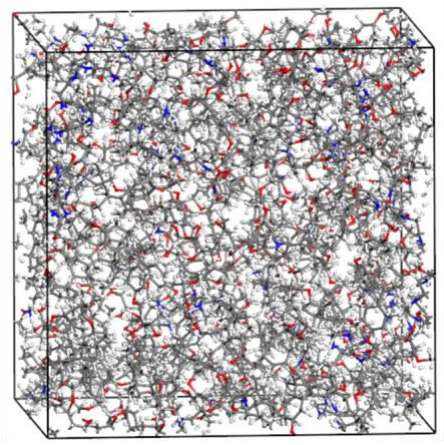

Figure 2: Simulation cell for the epoxy resin model with 90% crosslinking ratio by using 40 DETA and 100 DGEBA monomers.

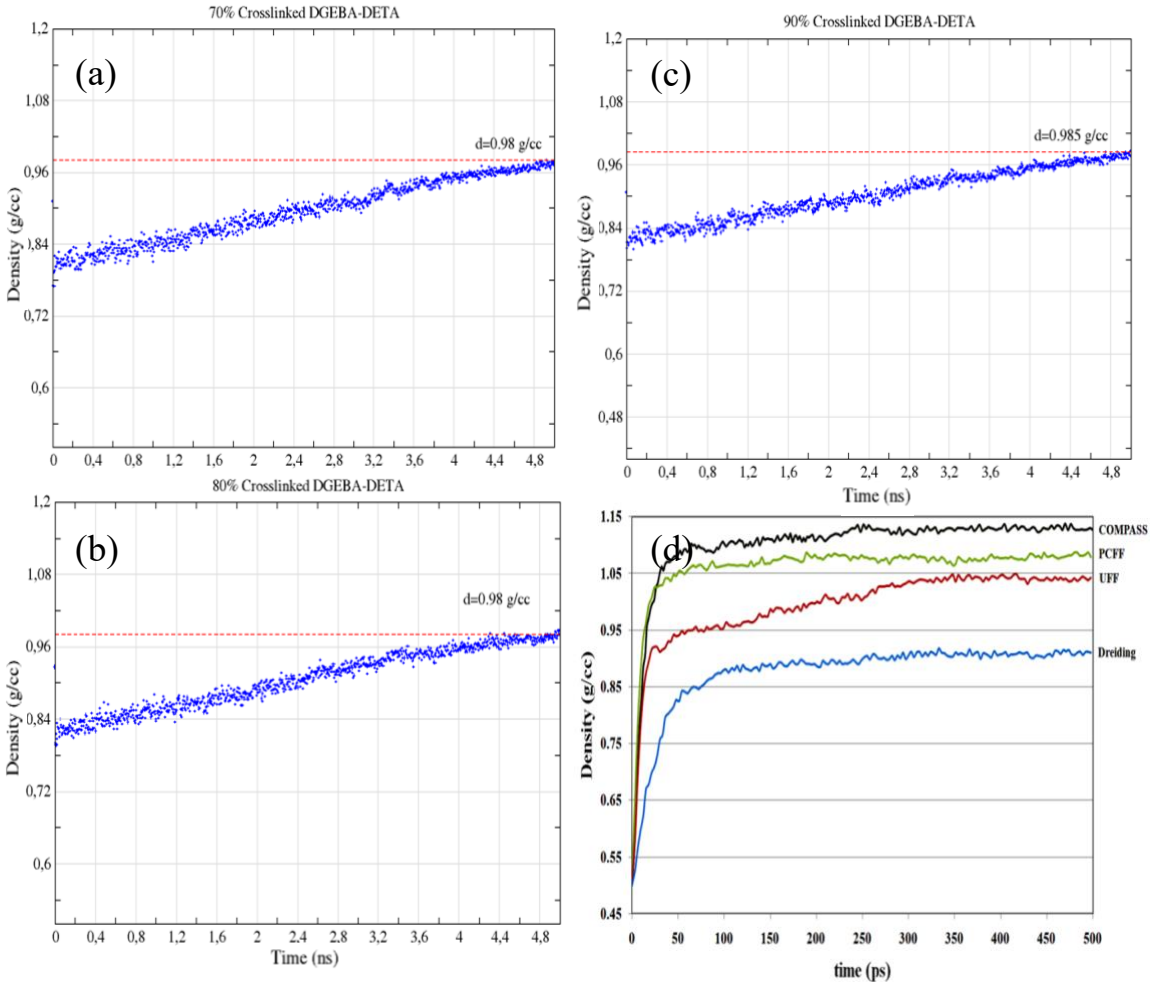

Figure 3: Equilibration of the density for crosslinked epoxy polymer with cross-linking degree (a) 70% (b) 80 % (c) 90 % using polymer consistent force field (PCFF) through 5 ns NPT dynamics. Each system cooled from 600 K to 298.5K (d) Equilibration of the density using different force fields through 500 ps NPT dynamics (Reference: B. Arab, A. Shokuhfar, J. Nano- Electron. Phys. 5 No 1, 01013 (2013))

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This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 951732. The JU receives support from the European Union's Horizon 2020 research andinnovation programme and Germany, Bulgaria, Austria, Croatia, Cyprus, the Czech Republic, Denmark, Estonia, Finland, Greece, Hungary, Ireland, Italy, Lithuania, Latvia, Poland, Portugal, Romania, Slovenia, Spain, Sweden, the United Kingdom, France, the Netherlands, Belgium, Luxembourg, Slovakia, Norway, Switzerland, Turkey, Republic of North Macedonia, Iceland, Montenegro