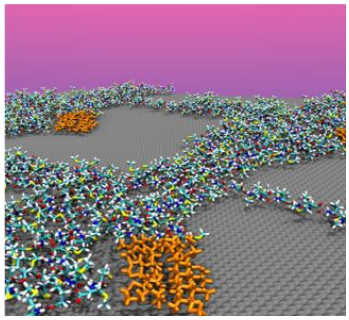
ARC LIEF GPGPU CLUSTER – IMPACT USE CASE SUMMARY

(Maximum 1 page – including an image)

TITLE: Predictions of Pattern Formation in Amino Acid Adlayers at the In Vacuo Graphene Interface: Influence of Termination State

BACKGROUND

The controlled self-assembly of biomolecules on graphene offers a pathway for realising high performance graphene-based nanodevices such as biosensors and biomedical implants. Despite the recognised importance of this control, the molecular-level factors that influence the self-assembly of biomolecules on graphene remain under-explored to date. This lack of fundamental insights impedes advances in bio-applications of graphene. These insights are challenging to obtain from experiment alone; molecular dynamics simulations provide a complementary approach to experiment in providing the required molecular-level details.



HOW DID GPGPU CLUSTER ENHANCE YOUR RESEARCH PROCESS

- In the research work, we modelled adlayers of amino acid/trace water on a graphene sheet in vacuo.
- The simulations were performed on the GPGPU cluster using the GROMACS/5.1.4-intel-2017.u2-CUDA module, which utilises the MPI architecture.
- The GPGPU cluster provided an ideal platform for the simulations as the GROMACS code supports gpu-accelerated multi-level hybrid parallelisation, thereby improving performance.
- For each job, 32 instances (ntask=32) of this program were run on multiple nodes, each using 1 core (cpus-per-task=1), with one requested GPU (gres=gpu:1).
- With these inputs, we obtained a performance of 0.89 ns/hr on the GPGPU cluster, which was estimated to be ~25% faster when compared to the performance obtained for an equivalent run on a comparable CPU-only cluster (0.71 ns/hr).

RESEARCH RESULTS

Based on the work that was supported by the LIEF HPC-GPGPU cluster, we reported, for the first time, the spontaneous emergence of dimer row ordering in adsorbed tryptophan and methionine adlayers on graphene, using all-atom molecular dynamics simulations. These patterns were consistent with scanning tunnelling microscopy data, and provided additional key insights that cannot be obtained from such experiments. The amino acid dimer row patterns only formed when charged termination states (zwitterions) were present in the adlayers. Adlayers containing only neutral states did not assemble into ordered patterns. Our research also showed that the presence of trace water in ultra-high vacuum reduces inter-amino acid interactions but does not induce or disrupt the spontaneous formation of patterns. Our findings reveal fundamental insights into the links between termination state and, both inter-amino acid interactions and amino acid-graphene interactions, that will enable advances needed to design the emergence and control of surface induced pattern formation of biomolecules. The design and control of surface induced pattern formation biomolecules will ultimately impact applications ranging from biosensors to functional nanomaterials for therapeutics. The outcomes of this work were recently published in Small (impact factor 10.9):

"Predictions of Pattern Formation in Amino Acid Adlayers at the In Vacuo Graphene Interface: Influence of Termination State", Joel B. Awuah and Tiffany R. Walsh, **Small**, early view https://doi.org/10.1002/smll.201903403

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