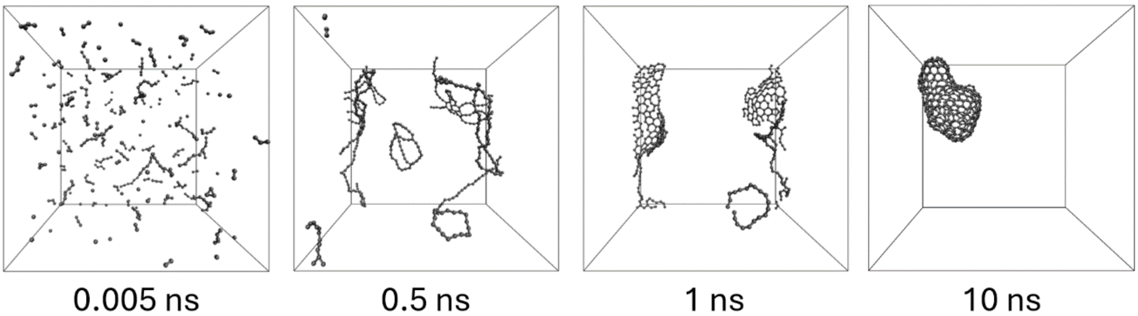
Foundation Models and Transfer Learning as Innovative New Routes for Atomistic Simulations of Low-Dimensional Carbon Materials

Christian L. Ritterhoff[a], **Yury Lysogorskiy**[b], **Anton Bochkarev**[b], **Ralf Drautz**[b], **and Bernd Meyer**[a]

[a] *Interdisciplinary Center for Molecular Materials (ICMM) and Computer Chemistry Center (CCC), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Germany*
[b] *Interdisciplinary Centre for Advanced Materials Simulations (ICAMS), Ruhr-Universität Bochum (RUB), Germany*

Machine-learned interatomic potentials (MLIPs) are rapidly transforming materials modeling by enabling quantum-accurate atomistic simulations on time and length scales that were previously out of reach. For the design and discovery of low-dimensional materials, these models could provide an unprecedented theoretical complement to experiments by allowing detailed insight into the thermodynamic and kinetic pathways governing their synthesis and transformation. The advent of foundation models extends this capability even further by covering wide regions of the chemical space in a single model. Refinement for a specific chemical configuration then allows the rapid exploration of previously inaccessible complex synthesis pathways. In this work, we fine-tune a graph atomic cluster expansion (GRACE) foundation model for carbon using the dataset by Qamar *et al.* [1] and subsequently distill its knowledge into a fast, local atomic cluster expansion (ACE) potential. This distilled model can efficiently capture the self-assembly of carbon clusters and the spontaneous formation of fullerene-like structures in dense inert-gas environments. These results illustrate how transfer learning and model distillation make foundation-model-based MLIPs a powerful new tool for studying the atomistic dynamics of nanostructure formation. As these models continue to incorporate richer chemistry and interfacial effects, they promise a new level of integration between theory and experiment in the understanding and controlled growth of 2D materials.



REFERENCES

[1] M. Qamar, *et al.*, J. Chem. Theo. Comput. **19** (2023) 5151–5167