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# Simulating Carbon Nanotube Growth with Machine Learning Force Fields


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## Date: Wednesday, October 9, 2024 14:30-16:00
## Venue: Faculty of Engineering Bldg. 2, Room 31A

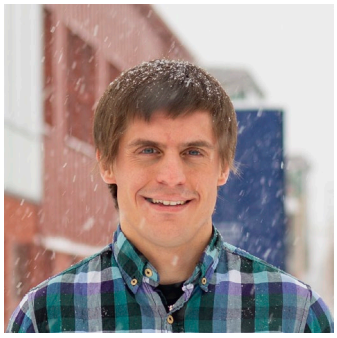

**Abstract:**

Carbon nanotubes (CNTs), hollow cylinders made of carbon atoms, are commonly synthesized through catalytic chemical vapor deposition using nanosized liquid catalysts such as iron, cobalt, nickel, or crystalline (solid) catalysts like rhenium or cobalt-tungsten alloys. Experimental studies have shown that liquid catalysts tend to produce broad chirality distributions, whereas solid catalysts result in narrower distributions, suggesting distinct CNT growth mechanisms. However, a detailed atomic-level understanding of these mechanisms has remained elusive from experiments alone.

Here, I will present our recent work using machine learning force field (MLFF) driven molecular dynamics (MD) simulations to model CNT growth on liquid Fe catalysts, as well as ongoing efforts to simulate growth on solid Re catalysts. MLFFs enables MD simulations with ab initio accuracy over microsecond timescales, allowing for simulations of the formation and continuous growth of long, defect-free CNTs.

For liquid Fe catalysts, the entire growth process was studied, from nucleation to growth including defect formation and healing. Simulations reveal a highly dynamic tube-catalyst interface with significant fluctuations in the CNT-edge chirality, because of high configurational entropy. Results show that defects form stochastically at the interface but are healed under low growth rates and high temperatures, enabling the growth of defect-free CNTs of considerable length. These findings, which are difficult to observe experimentally, highlight the power of MLFF-driven simulations in advancing our understanding of CNT growth.

For CNT growth on Re catalysts, preliminary results indicate that nanosized Re clusters remain crystalline at 1400 K, with well-defined facets and a hexagonal close-packed structure. Due to the low solubility of carbon in Re, carbon forms dimers and short chains on the catalyst surface, with diffusion rates varying across different facets. Some facets promote carbon transport, while others act as diffusion barriers. Simulations demonstrate CNT growth at 1400 K with a carbon supply rate of 100 carbon atoms per microsecond. These insights provide a deeper understanding of CNT growth mechanisms on solid catalysts and offer valuable guidance for controlled synthesis.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主催：
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