Contribution ID: **478** Type: **Poster**

M1Po3D-03: Assessing the Feasibility of Adopting Molecular Dynamics in Designing Cryogenic Polymers

Monday 19 May 2025 14:00 (2 hours)

Thermoplastics have long been a focal point in materials science, particularly in applications such as liquid hydrogen infrastructure and space fuel tanks. Their lightweight make them highly advantageous in such advanced technologies. However, the exploration of novel polymers for cryogenic applications has remained restricted to a limited subset of materials due to the high costs associated with experimental synthesis and testing. This limitation has hindered innovation, preventing the discovery of new monomers and the development of a molecular-level understanding of cryogenics-specific polymers. While computational approaches like Molecular Dynamics (MD) are well-established in fields such as drug design, their adoption in cryogenic polymer design remains underexplored, representing a missed opportunity for advancing cryogenic engineering.

MD offers a powerful method for simulating and characterizing the behavior of polymers at the atomic level. With the use of the Newtonian motion of atoms, MD provides critical insights into the mechanical, thermal, and permeability properties of materials, enabling the prediction of performance of polymers under cryogenic conditions. This study focuses on the simulation and analysis of polyetheretherketone (PEEK), a semi-crystalline polymer known for its exceptional mechanical and thermal properties as a case study to evaluate the adoptability of MD simulations in cryogenic polymer designing. MD simulations were used to examine key properties of PEEK at cryogenic temperatures, including tensile strength, Young's modulus, Poisson's ratio, coefficient of thermal expansion, and cryogenic hydrogen permeability, which are critical for cryogenic applications. Recognizing the semi-crystalline nature of PEEK, amorphous and crystalline phases were modelled separately. The simulations utilized two force fields: the Optimized Potentials for Liquid Simulations (OPLS) force field and the reactive force field (ReaxFF). For OPLS, CM5 charges were used as partial charges, derived from Density Functional Theory (DFT) calculations performed using the ORCA. This approach ensured high reliability in representing atomic interactions and charge distributions, thereby enhancing the accuracy of the MD results. MD simulations were run on Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). After equilibration, isothermal-isobaric ensemble (NPT) was used to examine the glass transition and melting temperature of the polymer which validates the ability of the MD simulations to capture polymer properties.
Also, this study presents the comparison of cryogenic experimental results of tensile strength, Young's modulus, Poisson's ratio, and coefficient of thermal expansion with the MD simulations providing insight on the possibility of using MD simulations in cryogenic polymer designing. Although molecular dynamics provide a significant amount of details at the atomic level, converting molecular scale results into macro-scale requires a multiscale modeling approach linking two distinct material levels. Therefore, finally, this study presents a comprehensive computational workflow that can be adopted in converting MD results for composite designing.

The findings of this research pave the way for broader adoption of computational chemistry techniques, especially MD in the field of cryogenic polymer composites. By integrating MD simulations and multiscale modeling, researchers can create a comprehensive toolkit for designing materials with unparalleled performance. As the demand for advanced materials in aerospace, energy storage, and hydrogen infrastructure continues to grow, molecular dynamics will enable revolutionizing the design and optimization of cryogenic polymers.

Author: COSTA, Susiri (The University of Melbourne)

Co-author: KRISTOMBU BADUGE, Shanaka (The University of Melbourne)

Presenter: KRISTOMBU BADUGE, Shanaka (The University of Melbourne)

Session Classification: M1Po3D - Insulation, Impregnation, and Polymeric Materials