Background and motivation - The performance properties of athletic wear have been driven by the development of new synthetic fibers such as polyesters. These offer numerous benefits including moisture wicking, better shape retention, and overall comfort. However, their use comes with drawbacks, including the retention of odor molecules found in human sweat (termed malodor molecules). This results in the phenomena known as ‘permastink’ – where sweaty smells persist even after repeated washing.

One of the prevailing theories is that the hydrophobic nature of synthetic fibers traps these molecules more strongly compared to cotton fibers which are made of cellulose. In addition, these molecules may not be removed during the washing process either because the molecules are trapped between the polymer chains prevented water from reaching them or they are more strongly bound to the chains compared to water. Other ideas on the causes of permastink have also been suggested including the growth of microbial colonies on clothing that survive washing (Herreweghen, 2020) or a combination of both (Munk, 2001).

Project Goals – To obtain a molecular level description of small molecule binding with textile polymers would provide powerful insight into how different malodor molecules might interact with the fibers. Specifically, the goal is to understand the types of interactions (e.g., hydrogen bonding) that drive binding of these malodor molecules to the fiber and whether the molecules interact with the surface of polymer fibers or are incorporated further into the fiber matrix.

Stages of the project work

Stage 1: Perform a literature review to decide whether you will need atomistic or coarse-grained models to use in simulations of the malodor molecules (the specific chemistries will be identified) and polyester (PET) system [Ref. The team may want to use (Zheng, 2022, 15(6)) as a starting point]

Stage 2: Run simulations to study interactions between isolated malodor molecules (3 or 4 types from the list of chemistries provided) and the polymer chains (in fibrillar configuration)

Stage 3: Run simulations to study clusters of molecules (nanodroplets) interacting with the polymer chains in fibrillar configuration.

Stage 4: Study how interactions between malodor molecules – polyester chains change with introduction of some humidity (water molecules).
**Expected skills** i) Molecular modeling and simulations ii) Familiarity with chemical engineering thermodynamics, fluids, transport phenomena iii) Polymer chemistry

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**Bibliography**

