Carbon nanotubes (CNTs), i.e., tubules of nano-diameter and walls made of a hexagonal network of carbon atoms, are characterized by unique electrical, thermal and mechanical properties, which would be highly desirable in the formation of various types of electrical conductors. There are many possible ways in which the nanotubes may be assembled to form macroscopic conductors. Unfortunately, their unique properties are then mostly lost. It has been recently theorized that properly structured CNT fibers (kilometers-long and micro-thin yarns made of axially aligned carbon nanotubes – Figure 1 a) could overcome this issue and transfer the unique thermal, electrical, and mechanical properties of individual CNTs into macroscale. Extensive experimental studies conducted around the world indicate that the best results in this respect are currently obtained via coagulation spinning of the fibers from liquid crystal CNT suspensions. The major drawback of this method is the necessity of using superacids which are hazardous and toxic.

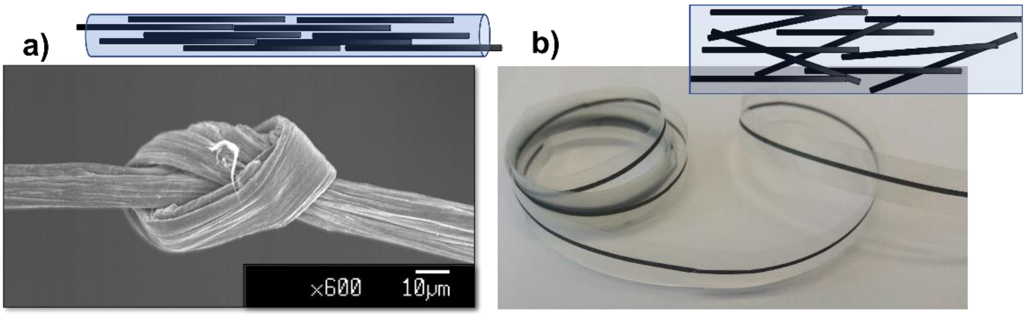

Fig. 1. a) CNT fiber and a drawing of its CNTs alignment. **b)** Printed CNT pathway and a drawing of its in-plane CNT alignment.

The aim of the current project is to undertake both experimental and modeling approaches to develop scalable methods of manufacture of acid-free liquid crystals, which may be further used for spinning CNT fibers. To obtain this goal, the PI would like to combine her unique experience working with CNT fibers gathered abroad, and the methodology of manufacturing conductive pastes and inks for printed electronics applications developed at the Warsaw University of Technology (Fig 1 b). The experimental research will include testing various solvents of high boiling point used for the formation of screen printing pastes, choice of matching coagulants, and use of different types of nanotubes (changing length, number of walls, chiralities). The studies will also investigate potential methods enabling scale-up of the manufacture of acid-free CNT liquid crystals and small-scale spinning of CNT fibers.

To better understand the given system and reduce the experimental efforts in finding the best components (solvents, coagulants), the project will be realized in collaboration with Dr. Karolina Milowska (Ikerbasque Research Fellow - CIC nanoGUNE, Spain), who will co-supervise the Ph.D. student and take the lead on the modeling part of the project. In this part of the project, first principles modeling (DFT - density functional theory, DFTB - tight binding method based on DFT) and molecular dynamics and Monte Carlo simulations using reactive force fields will be undertaken. This modeling will help explain the interaction mechanisms between nanotubes and solvent molecules. On the other hand, simulations using reactive force fields will make it possible to explain their interaction on a larger scale and the dynamics of this interaction while maintaining the accuracy of DFT calculations. Monte Carlo simulations, in particular, will extend the time scale.

The obtained research results are expected to significantly advance the studies on the formation of highly conductive CNT fibers. Simultaneously, they are also expected to be of paramount importance for improving the performance of less conductive but inexpensive and highly versatile printed CNT conductors.