Between 29th January and 4th May 2018, I spent three months on a placement at Dassault Systèmes BIOVIA in Cambridge. DS BIOVIA provide software solutions that help science-driven companies create innovations in chemicals, pharmaceuticals, and materials industries. During my internship, I worked with the Materials Studio development team – Materials Studio is a software package that combines a vast variety of simulation tools for calculations and modelling in materials science and chemistry. It provides a multifunctional toolbox that accurately predicts structures of molecules and crystals, chemical reaction pathways, and spectroscopic properties of materials.

My project revolved around the atomistic simulation of lithium-ion batteries, in the context of developing more efficient power sources for the next generation of electric vehicles in the automotive industry. The first phase of my placement focused on density functional theory (DFT) calculations of lithium transport, aiming to understand the transport mechanisms in battery electrodes at different concentrations of lithium ions. During the second phase, my role shifted towards software development and improving a Monte Carlo simulation code included in Materials Studio. In particular, I have implemented new functionality for extracting the diffusion rates from the quantum mechanical DFT data I obtained in the first part of my project.

During the three months at DS BIOVIA, I had an amazing opportunity to be immersed in the rich and diverse field of computational materials science, and get my first experience working in a commercial software development environment. Equally important was the great company culture and I had excellent mentoring arrangements – including an opportunity to talk to colleagues from different departments and gather insights about their career paths and various aspects of their day-to-day work.

My placement at DS BIOVIA was truly a mind-opening experience, which gave me a fresh perspective on the career trajectory I would like to follow after my PhD. I highly recommend taking advantage of the CM-CDT industrial placement scheme to anyone in the CDT.