Kinetic Monte Carlo (kMC) is a stochastic method used to simulate time evolution of a system. This algorithm finds application in various scientific fields. It is also widely used in physics of thin films. In the thesis, we developed models based on the kMC method to simulate growth and electronic properties of thin film.

First, we developed the model to simulate the pulsed-laser deposition (PLD) growth of multiferroic perovskite. The model was first validated with data from literature and then used to clarify some of the phenomena observed during PLD growth.

We innovatively explained the inter-layer transport crucial for film morphology using natural configuration-based processes. In addition, we were able to identify the cause of the experimentally observed decrease of surface roughness with increasing laser frequency.

Second, we used the kMC method to study polaron diffusion with the aim to further understand the charge transfer in doped hematite. We applied several approximations of how dopants could affect the charge transfer and found that they influence polaron diffusion globally rather than due to strong local effects. Moreover, our model suggests that the diffusion process depends on the polaron type. We also simulated the injection of hole polarons into doped hematite. Even using the general simulation setup, we were able to reproduce the measurements made during the injection process.