Josephson junctions are key components of quantum computers based on superconducting qubits. Although superconducting qubits are one of the most promising candidates to realise large-scale quantum computing, the materials science of Josephson junctions still limits their performance. Imperfections in Josephson junctions fabricated today are a source of energy dissipation and decoherence, as well as parameter drift and uncertainty. A possible explanation for this energy dissipation is the presence of microscopic metallic links called “pinholes” that might exist within the oxide tunnel barrier in the device. Employing molecular dynamics and a tight-binding description of the system, we develop an atomistic model of Al/AlO\textsubscript{x}/Al Josephson junctions [1] as a method to resolve pinholes in the oxide tunnel barrier. Pairing this with a non-equilibrium Green’s function (NEGF) approach we study quasiparticle transport through the device [2] to understand how pinholes might affect current. We additionally use a Bogoliubov de-Gennes (BdG) description of the system to study transport properties of the device in its superconducting state to understand how defects in the junction may affect the current-phase relationship in the device [3].

Figure 1: An atomistic Al/AlO\textsubscript{x}/Al Josephson junction constructed using molecular dynamics.