Simulation of scanning tunneling microscopy from first principles

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Abstract

Since its invention in the early 1980's scanning tunneling microscopy (STM) contributed to the rapid development of nanoscience and nanotechnology, and has been actively used in many subfields of surface science to study a wide spectrum of materials' surfaces.

In my research I focused on developing and implementing computationally efficient electron tunneling models for the simulation of high-resolution STM and SP-STM images. These models are based on first-principles electronic structure calculations and capable of handling arbitrary tip orientations. My research contributes to the highly complex task of interpreting experimental STM images.