# Simulating X-STM images of iso-electronic dopants in semiconductors using DFT

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The sizes of devices and active regions in semiconductor devices are reaching the atomic scale. This requires us to have an understanding and control over defects at this level as well. A technique that is very well suited to investigate semiconductors at this scale is Cross-Sectional Scanning Tunneling Microscopy (X-STM). We employ this technique to study iso-electronic dopants in III-V semiconductors. We study these dopants since they can locally modify band gaps and other electronic characteristics of a semiconductor which makes them interesting for device fabrication. These X-STM images that we generate can be difficult to interpret however, since the Local Density of States (LDOS) of a material is probed rather than the topology of the material surface alone.
For this reason we combine this experimental technique with Density Functional Theory (DFT). We have developed a method to simulate LDOS planes above a surface supercell which can be more directly compared to the X-STM images we generate. This can help us understand the underlying topology of the X-STM images as well as helping us understand what it is that we are seeing when starting X-STM measurements on unknown materials or dopants.
This combination of techniques is applied to three different doped materials: N doped InAs, B doped GaAs and Tl doped GaAs. The N doped InAs and B doped GaAs were used to test the technique since a lot of data about both of those systems studied with X-STM is available. [1] The Tl doped GaAs however, is a material which is not measured before with X-STM and therefore the DFT simulations have helped with the interpretation of the X-STM data. In all three cases we find a strong correspondence between the X-STM and DFT results as seen in Figure 1.

[1] Verstijnen, T. J. F., Tjeertes, D., Banfi, E. G., Zhuang, Q., & Koenraad, P. M. (2023). Atomic scale analysis of N dopants in InAs. *Physical Review B*, *108*(4), 045302.

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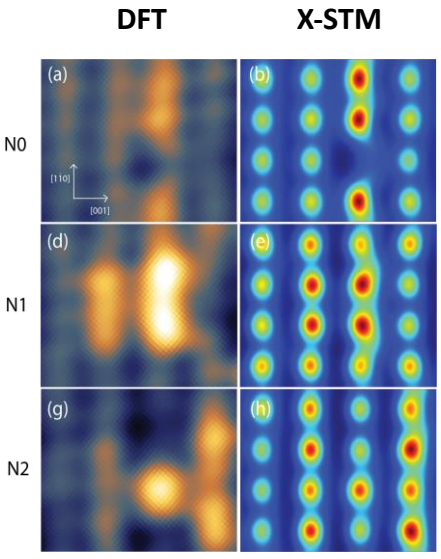


Figure 1: Comparison between DFT simulations and X-STM data for N doped InAs