We offer a Masters' / Bachelor's project with an open starting date on

Advanced simulations of electron holographic mean inner potentials

Summary

Nanoscale electric potentials can be investigated using electron holography in the transmission electron microscope. However, full quantification often relies on knowing the mean inner potential V_0, defined as the electric potential difference between the interior and the exterior of a material. Unfortunately, V_0 has been difficult to accurately and precisely measure experimentally, with many measurements disagreeing with each other. Recently, density functional theory (DFT) simulations have emerged as a predictive tool, indicating i.a. the possibility of strong surface-condition effects. However, DFT simulations of V_0 have only been used for a few materials. Applying these techniques to additional materials can help guide future research.

This project will investigate V_0 for different materials using ground-state DFT under a range of conditions. This project is primarily computational.
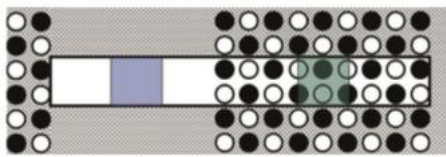
Figure 1: Thin-slab geometry used for V_0 calculations, by taking the average DFT-generated potential in the green area and the blue area.
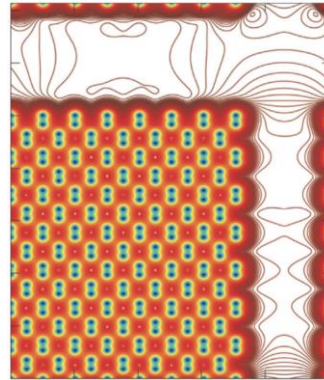

Figure 2: Fringing fields outside a bulk-like nanowire, calculated using DFT. This may help explain V_0 surface facet dependence.

Figures from R. S. Pennington, C. B. Boothroyd, and R. E. Dunin-Borkowski, Ultramicroscopy **159**, 34 (2015).

The student should have these skills:
- Knowledge of Matlab or Python, macOS or Linux
- Competence in English communication (written and spoken)

The student should learn the following:
- Basic familiarity with Python for scientific applications
- Ground-state atomic-scale density functional theory
- Elementary transmission electron microscope applications
- Scientific writing and communication in English

If interested, please contact:
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