

Factors Affecting Measurements of Semiconductor Mean Inner Potentials

Robert S. Pennington*^[1], Jens J. Mortensen^[2], Takeshi Kasama^[1], Chris Boothroyd^[1], Rafal E. Dunin-Borkowski^[1]

[1]: Center for Electron Nanoscopy, Technical University of Denmark
[2]: Center for Atomic-Scale Materials Design, Technical University of Denmark
* Corresponding author: robert.pennington@cen.dtu.dk

Introduction

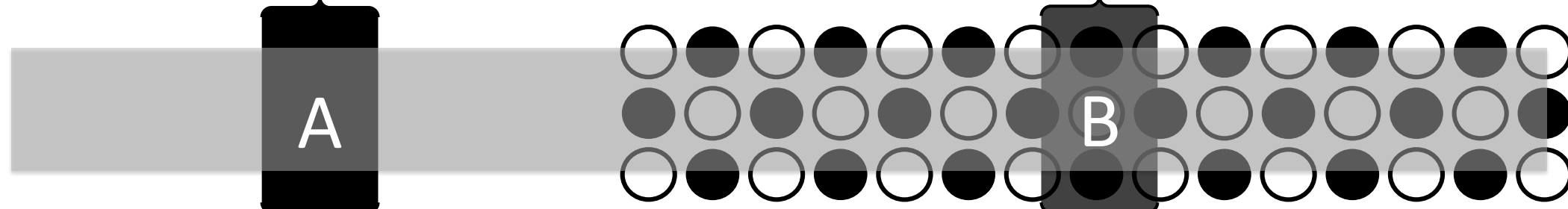
The mean inner potential (MIP) is of interest for electron holography, where it affects the measured phase^[1]. But, there is large variation in experimental measurements of the MIP. Therefore, calculations may provide guidance on interpretation of experimental measurements, especially on the role of the surface. In this work, we use density functional theory to calculate mean inner potentials of semiconductors. The stability of the simulator with respect to calculation parameters is found. These conditions are then used to simulate the mean inner potential for silicon under different surface conditions, including surface facet, adsorbates, and surface reconstruction. The effect of diffraction contrast on phase profiles of nanowires is also examined experimentally.

Density Functional Theory and GPAW

Density functional theory (DFT) allows for the calculation of electronic structure. The grid-based projector-augmented wave method, implemented as the GPAW simulator by CAMd at DTU, allows for real-space calculation of the electron density^[2]. This allows for convenient mean inner potential calculations.

Calculation Geometry

Objective: Use calculation geometry that allows MIP calculations.



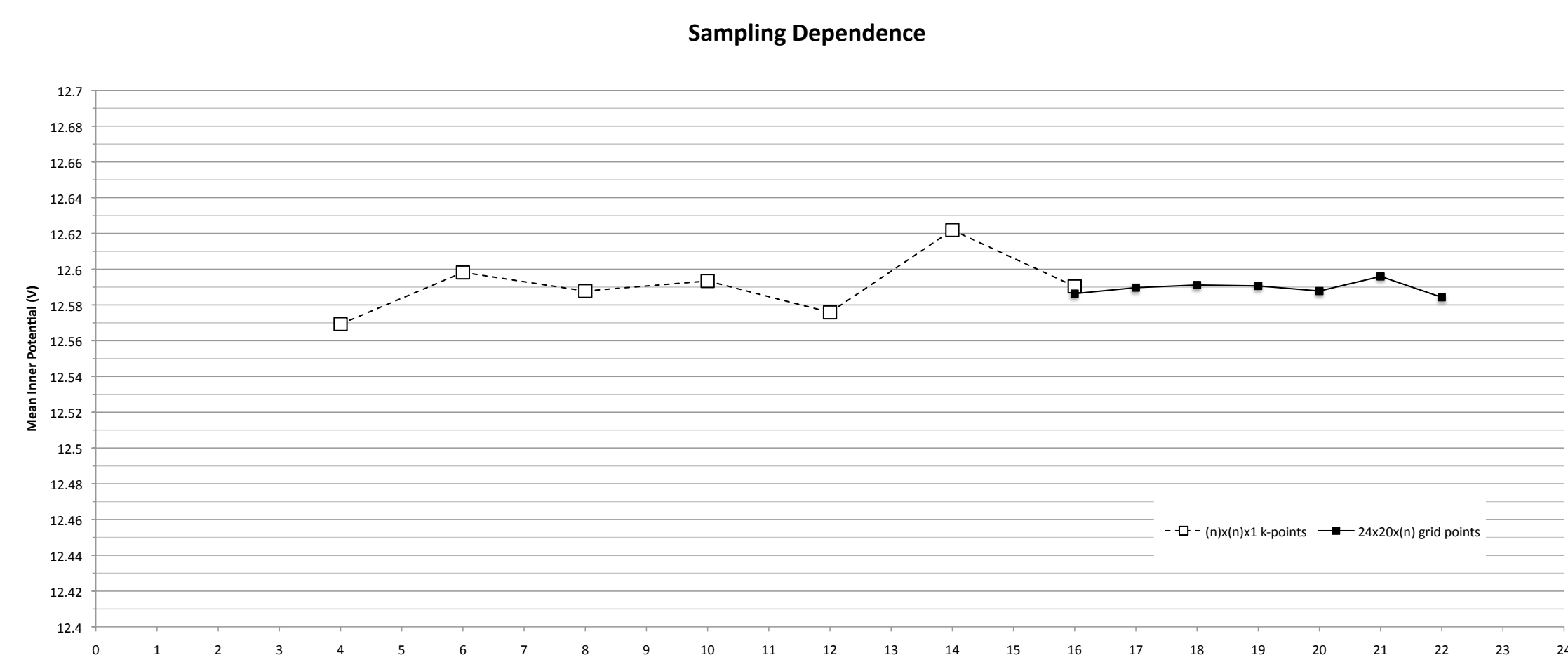
The MIP calculation requires the potential in a region of vacuum, labeled A, to be compared to the potential in a region of material, labeled B. With the (110) direction normal to the surface, the surfaces of zincblende compound semiconductor slabs are nonpolar. This is the same calculation geometry used elsewhere^[3].

Verification of Simulator

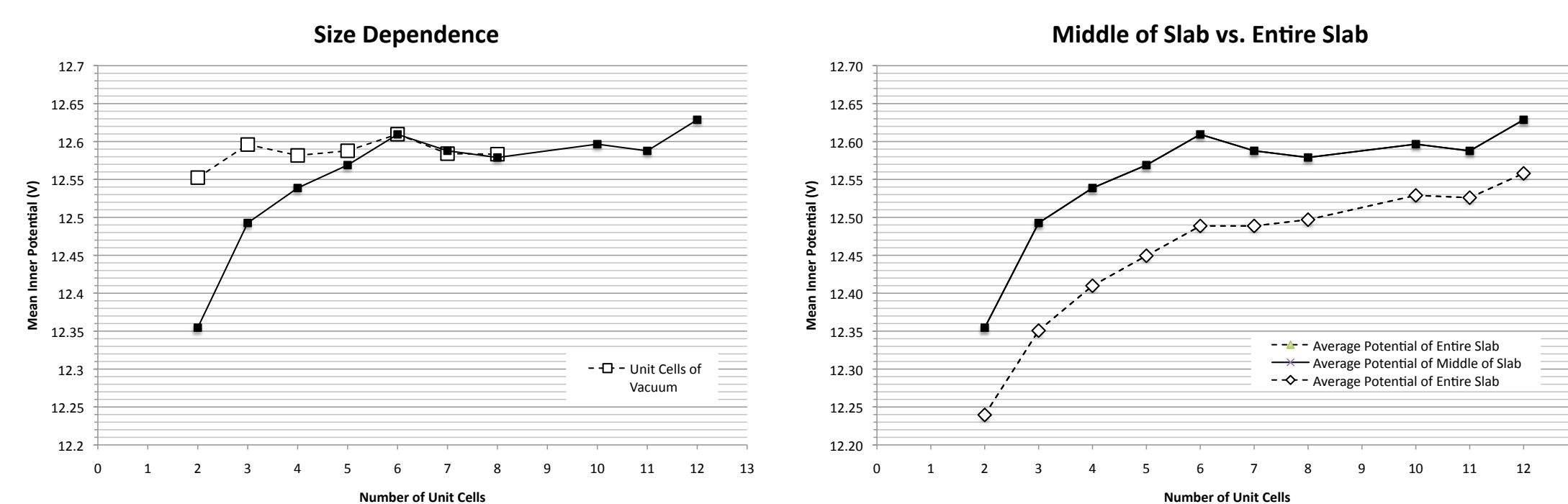
Objective: Verify that calculations of the MIP vary little when calculation parameters are changed.

Functional	MIP (V)
LDA	12.59
PBE	12.59
RPBE	12.61
revPBE	12.58

The MIP was relatively independent of exchange-correlation functional. The PBE functional was used as standard.



The MIP shows a low dependence on sampling density. Increasing numbers for both k-space and grid spacing indicate higher sampling and increased computation time. For stability, there must be an integer number of grid points per unit cell in the z-direction.



Variation of number of unit cells of Si and vacuum. Thinner Si slabs led to lower calculated mean inner potentials, while the number of layers of vacuum had minimal effect. 7 unit cells of Si, corresponding to 30 atoms, and 5 unit cells of vacuum were used as the standards.

The average potential in the center of the slab versus the average potential of the entire slab. The latter would correspond to the total phase shift experienced by an electron passing through the slab, and is consistently lower as a result of surface effects.

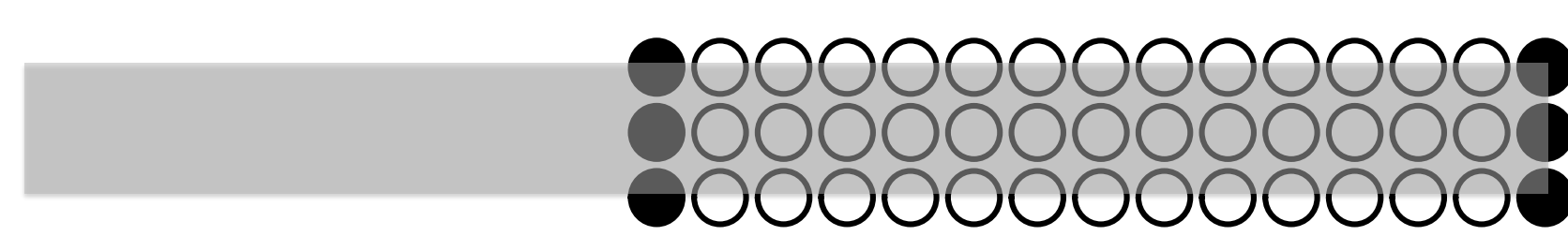
Calculated Mean Inner Potentials

Objective: Calculate MIP material and surface dependence.

Surface	MIP (V)
Si(110)	12.59
Si(100)	12.91
{2x1 recon}[6]	{12.32}
Si(111)	12.63
Si(211)	12.64

Even though the mean inner potential is measured in the middle of the slab relative to vacuum, adsorbate element and position have a measurable effect. Adsorbates were placed as seen below, and allowed to relax. White atoms are Si, black atoms are adsorbate.

Surface	MIP (V)
Si(all relaxed)	12.52
Si(C)	14.12
Si(C-relaxed)	12.01
Si(Ge)	12.46
Si(Ge-relaxed)	12.53



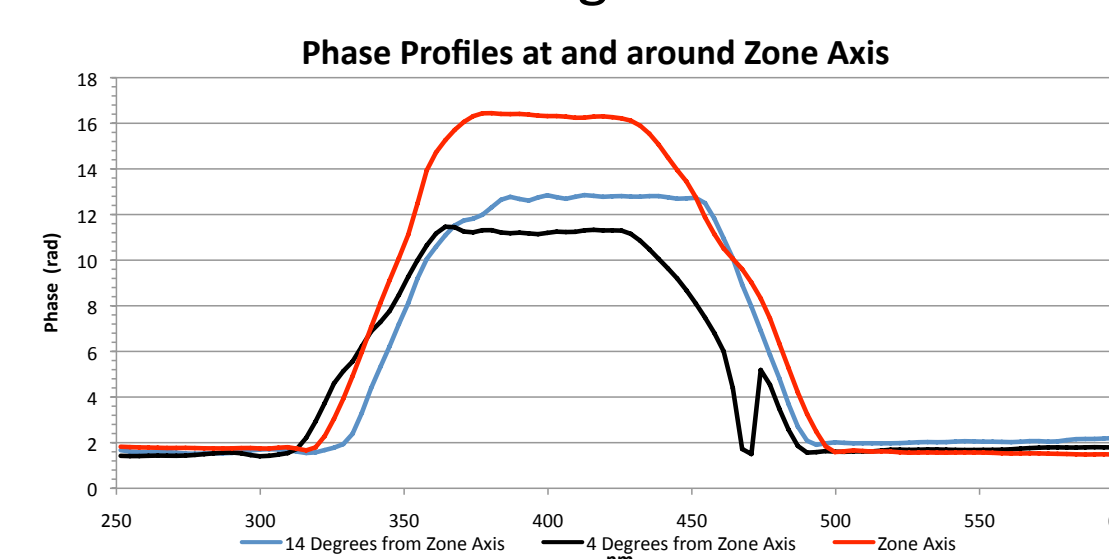
The chosen surface facet affects the MIP. The difference between (100) surfaces with and without a (2x1) reconstruction is 0.59V, but the differences between other surface facets are smaller [$<0.05V$].

Material	MIP _{DFT} (V)	MIP _{rel} (V)
Si	12.59	13.76
Ge	14.69	15.60
AlP	11.40	13.42
AlAs	12.29	13.97
GaP	13.57	14.60
GaAs	14.15	15.38
InP	13.85	15.22
InAs	14.13	15.47
CdS	13.02	13.87

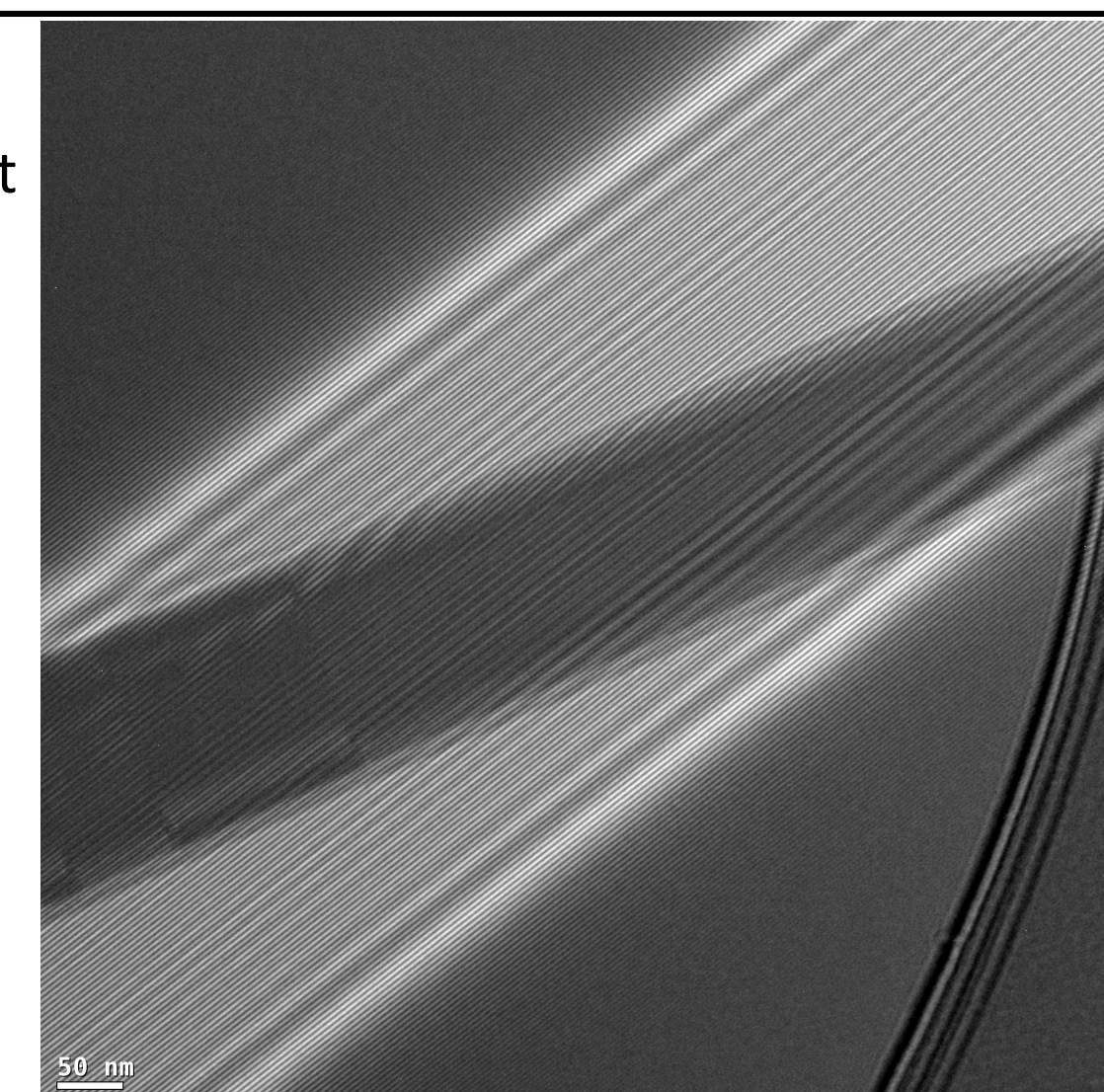
The MIPs calculated here are consistent with literature values for DFT calculations of these materials^[3]. The substantial difference between the result from DFT calculation and the results from electron scattering factors^{[4][5]} indicates the importance of electronic structure for MIP calculations.

Electron Holography

Objective: Examine how diffraction contrast affects electron holograms.



Line profiles across cross sections of reconstructed phase images taken at different tilts from zone axis. The nanowire was tilted about its long axis, so the thicknesses and phase changes should be similar; they are not, due to contributions from diffraction contrast.



Hologram taken at zone axis of GaAs nanowire.

Mean inner potential measurements would depend strongly on crystallographic orientation.

Conclusions & Further Work

Conclusions: We have calculated mean inner potentials of both compound and elemental semiconductors. Surface morphology and composition both affect the mean inner potential in the middle of the slab. Diffraction contrast can affect holograms and, therefore, the mean inner potential measured.

Further Work: Further work on calculations of mean inner potential should explore the effects of surface orientation and composition mindful of both stoichiometry and atom positions. Further experimental work should examine ways of determining the mean inner potential of a material with known atom positions.

References:

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