Efficient first principles simulation of electron scattering factors for transmission electron microscopy

Electron microscopy is a powerful tool for studying the properties of materials down to their atomic structure. In many cases, the quantitative interpretation of images requires simulations based on atomistic structure models. These typically use the independent atom approximation that neglects bonding effects, which may, however, be measurable and of physical interest. Since all electrons and the nuclear cores contribute to the scattering potential, simulations that go beyond this approximation have relied on computationally highly demanding all-electron calculations. Here, we describe a new method to generate ab initio electrostatic potentials when describing the core electrons by projector functions. Combined with an interface to quantitative image simulations, this implementation enables an easy and fast means to model electron scattering. We compare simulated transmission electron microscopy images and diffraction patterns to experimental data, showing an accuracy equivalent to earlier all-electron calculations at a much lower computational cost.

General information
Publication status: Published
Organisations: Theoretical Atomic-scale Physics, Department of Physics, University of Vienna, Ulm University
Corresponding author: Susi, T.
Number of pages: 7
Pages: 16-22
Publication date: 2019
Peer-reviewed: Yes

Publication information
Journal: ULTRAMICROSCOPY
Volume: 197
ISSN (Print): 0304-3991
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
Original language: English
Keywords: 2D materials, DFT, QSTEM, TEM
DOIs:
10.1016/j.ultramic.2018.11.002
Source: Scopus
Source-ID: 85056794497
Research output: Contribution to journal › Journal article – Annual report year: 2019 › Research › peer-review