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.

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