Factors of Atomic Electron Scattering (FAES): A resource for Gaussian parameterization of integral ionic, fractionally charged, and neutral electron scattering factors

Ambarneil Saha¹, Madeline Evans², Thomas Holton³, Jose Rodriguez⁴ ¹University of California, Los Angeles ²UCLA, ³UCLA, ⁴UCLA asaha@chem.ucla.edu

Electrostatic potential maps derived from cryo–EM can contain a wealth of information about charged states. However, access to such information is obstructed by the absence of appropriately parameterized ionic electron scattering factors. Existing parameterizations remain either incomplete or incompatible with least-squares refinement programs. To rectify this, we introduce FAES (Factors of Atomic Electron Scattering), a web server publicly accessible at <https://srv.mbi.ucla.edu/faes/>. This resource supplies Gaussian parameterizations of elastic electron scattering factors into three forms and calculates fractionally charged scattering factors by computing linearly weighted sums of adjacent integral neighbors. Using atomic scattering amplitudes tabulated in the International Tables for Crystallography, FAES provides numerical fitting coefficients, statistical goodness-of-fit values, and accompanying visual plots for all supported fits. We also derive elastic and estimated inelastic crosssections from FAES parameterizations at a range of accelerating voltages relevant to transmission electron microscopy.