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【222】 Vienna Package for TensErLEED I: A new environment for analysis and calculation of LEED $I(V)$ data

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Low-Energy Electron Diffraction (LEED) is a structure-sensitive technique commonly used to determine periodicity and order of a surface phase. Quantitative analysis of the modulation of beam intensities as a function of voltage (LEED $I(V)$) also gives access to the surface atom positions. This requires complex calculations and optimization of structural parameters. The Erlangen program package TensErLEED readily performs this task, but its required user input is prohibitively complex.

We introduce the new “Vienna Package for TensErLEED” (ViPerLEED), which greatly simplifies the use of TensErLEED, only requiring a standard structure file and a handful of user parameters. The package also includes a utility for extracting experimental $I(V)$ spectra from LEED videos.

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