Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

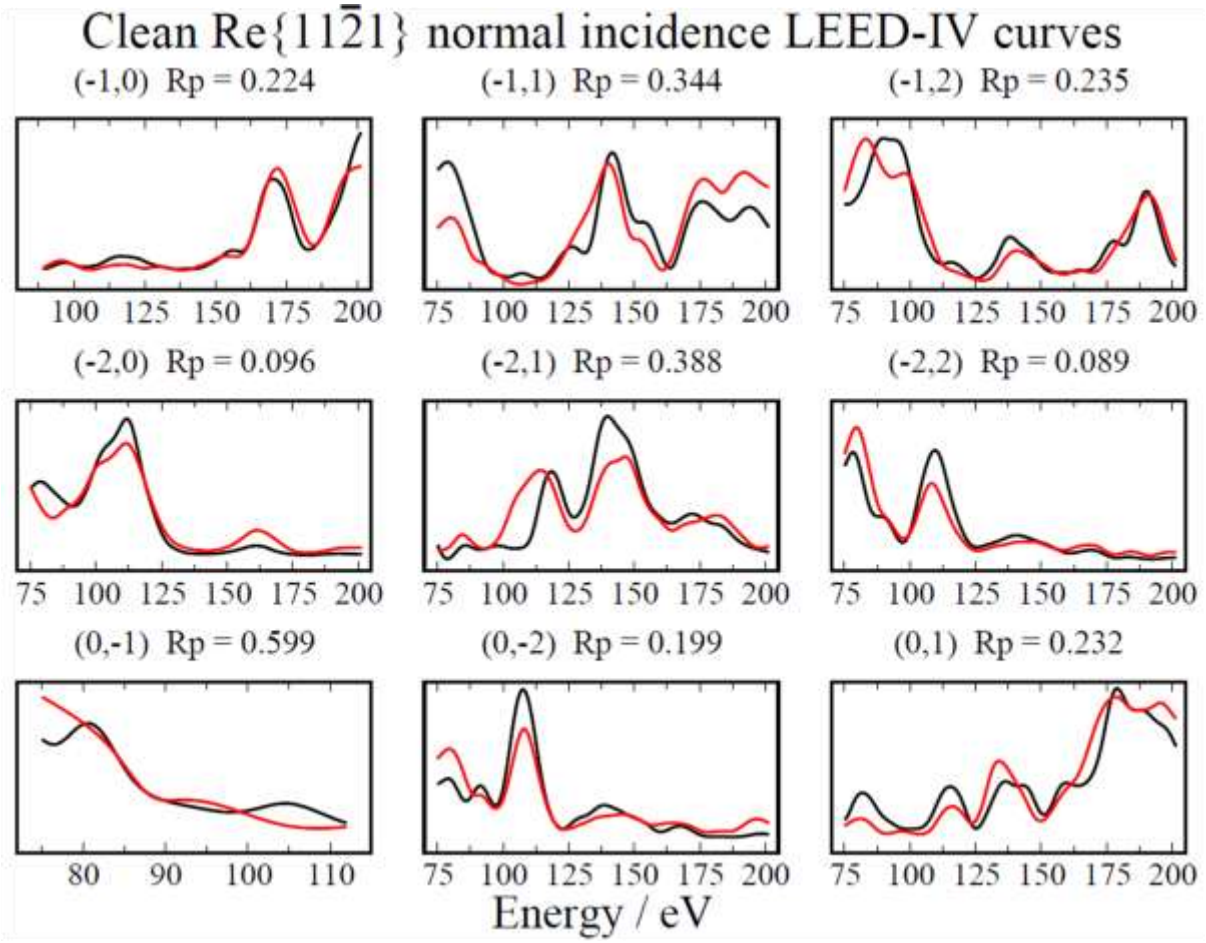
Supplementary Information

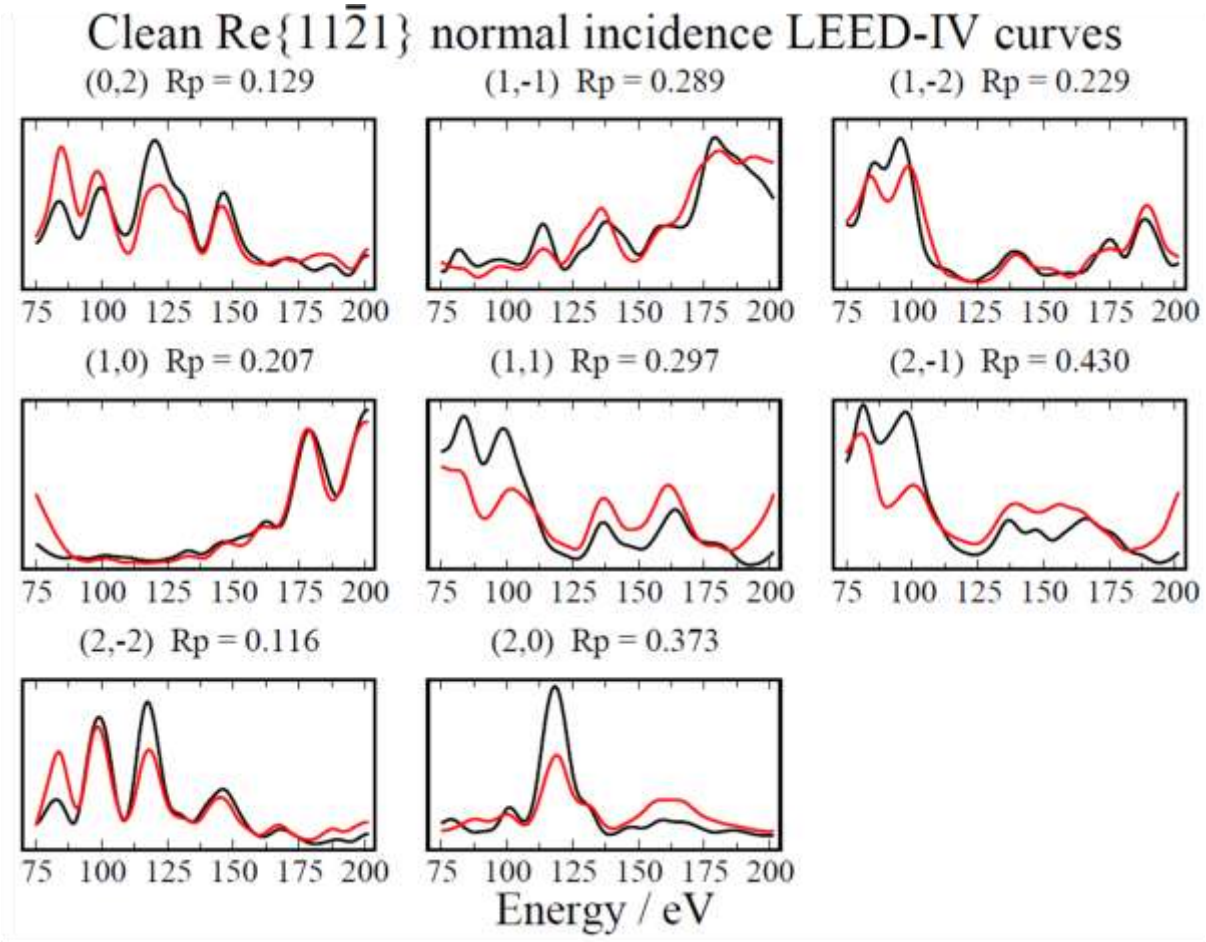
LEED-IV Calculations

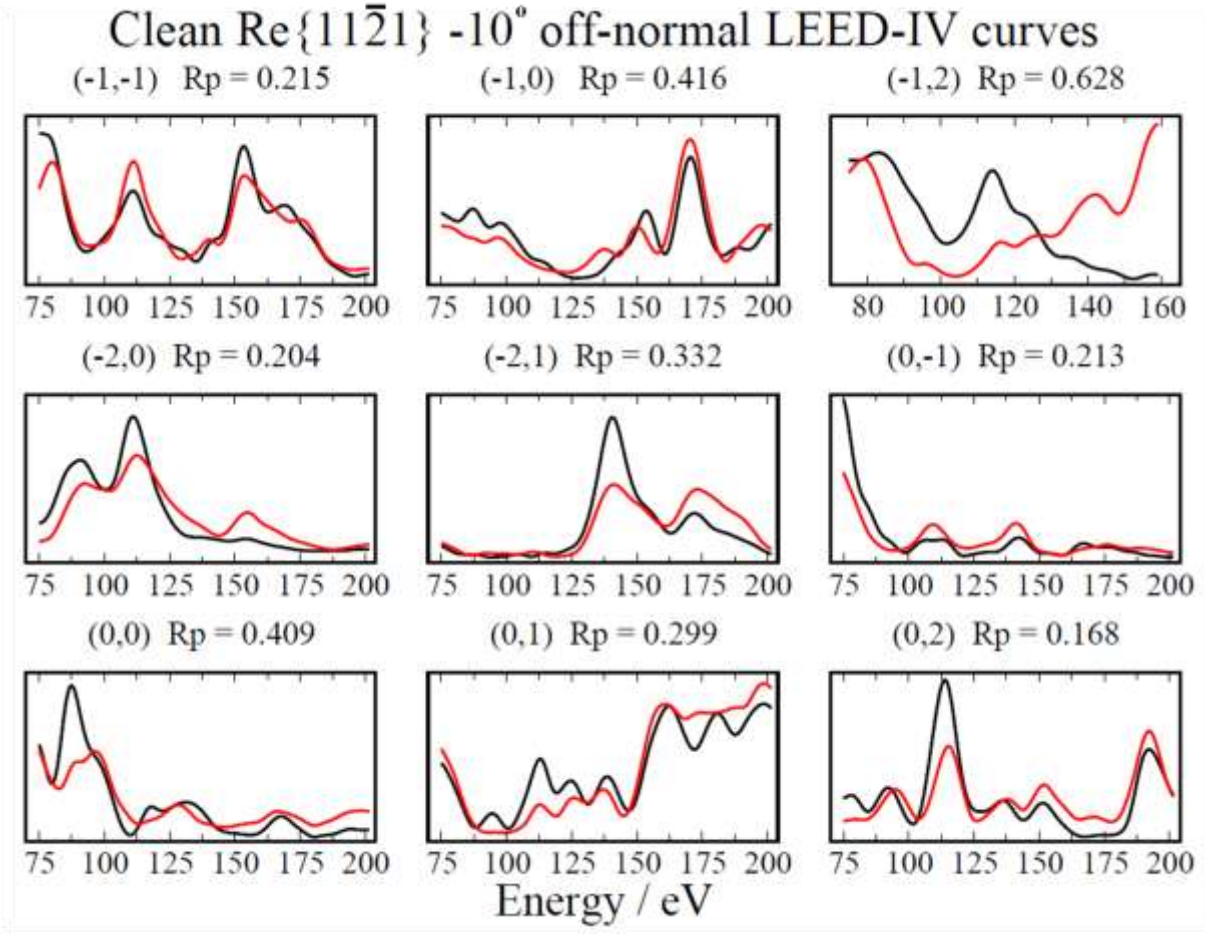
The combined space or "giant matrix inversion" method [1] was employed to perform the LEED-IV calculations for this surface due to the small interlayer spacing of 0.659 Å. Scattering phase shifts for Re atoms were calculated as a function of energy using the program package provided by Barbieri and Van Hove [2]. The maximum angular momentum quantum number was set to 9. The imaginary and real parts of the inner potential were set to 4.72eV and -13.1eV. Initially, the radial root mean square displacement for Re were assumed to be 0.08Å. In the final stage of the searches the displacements were optimized together with the inner potential to obtain the best fit between theory and experiment. The downhill simplex method was used for the structure optimization[2]. RR is the reliability of the R-factor (R_P), $RR = \sqrt{\frac{8V_i}{\Delta E}}$, where V_i is the optical potential and ΔE is the total energy range analysed.

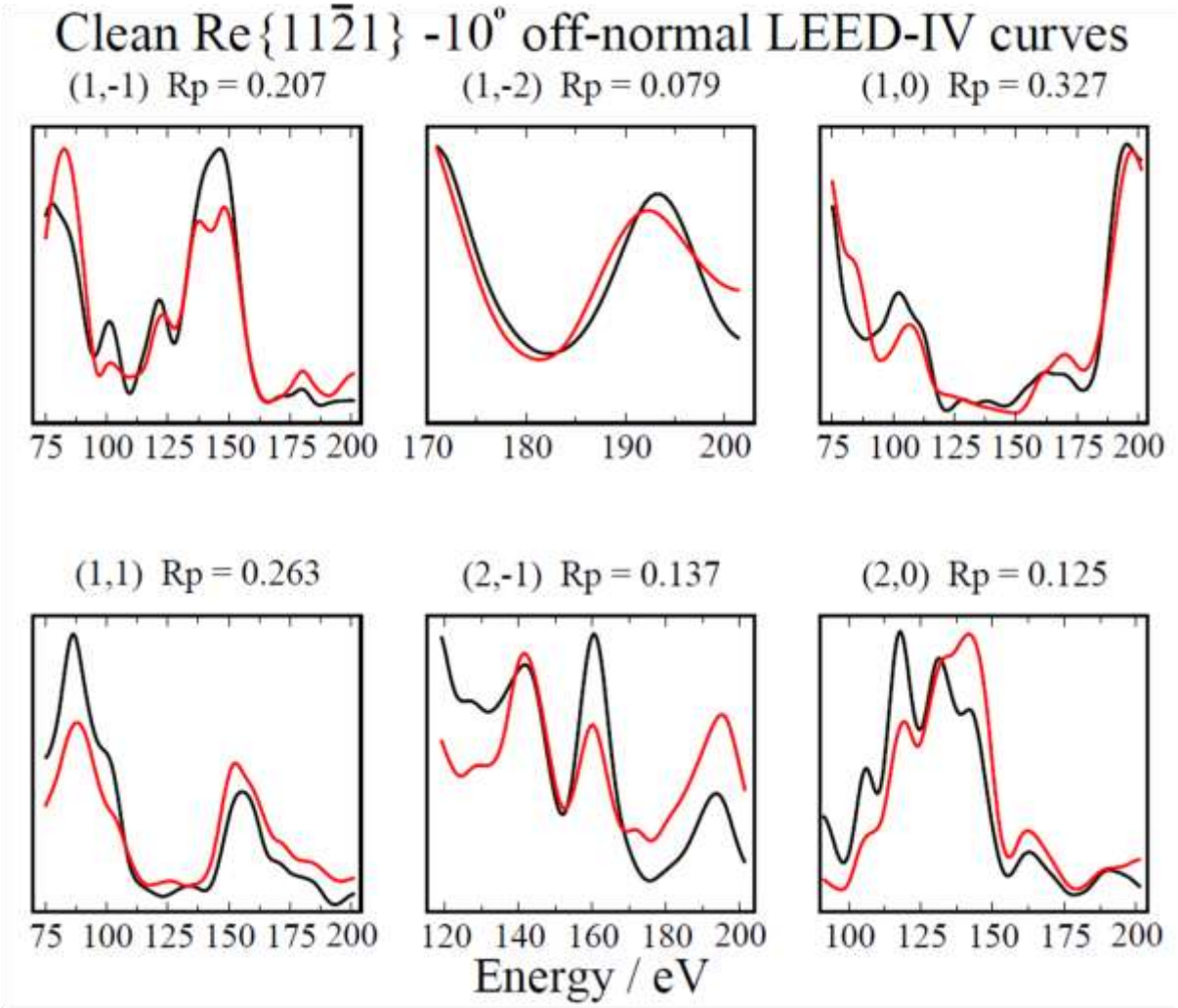
LEED-IV Figures

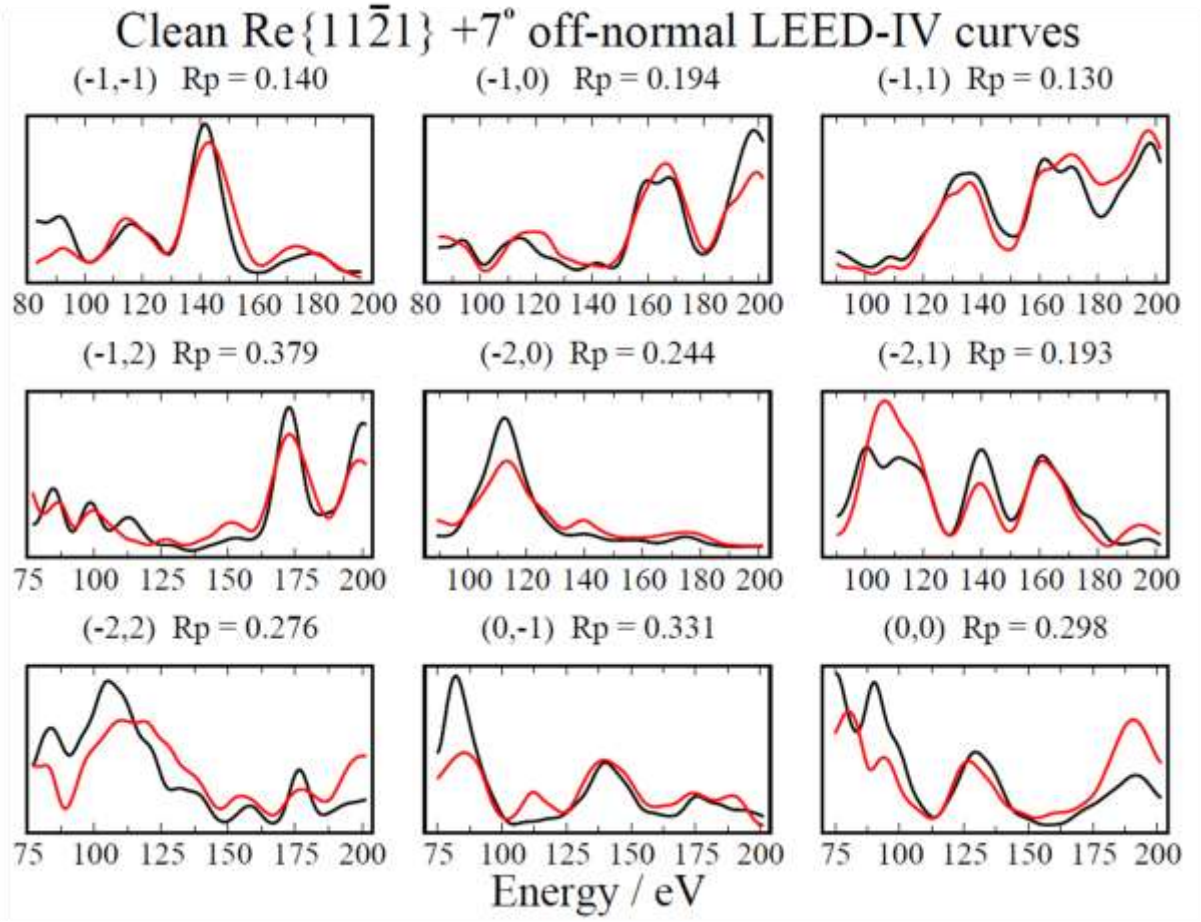
The full set of LEED-IV data and best fit curves are given in the following sets of images. For each the title is self explanatory and the black curves are the data and the red curves are the best fits. Individual R_P values are indicated for each fit.

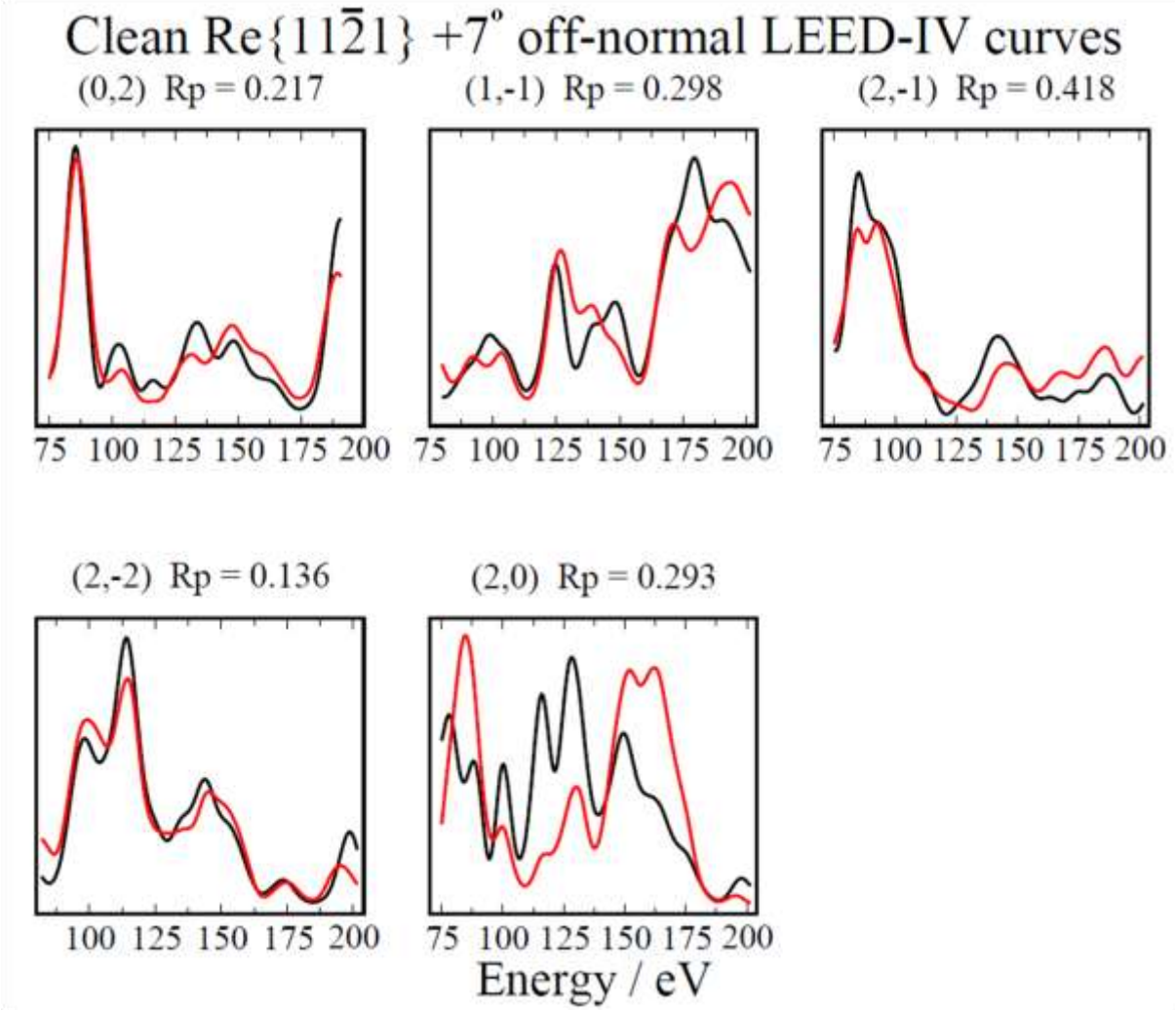












[1] M. A. Van Hove, W. H. Weinberg, and C. M. Chan, *Low Energy Electron Diffraction* (Springer, New York, 1986)

[2] Barbieri, A.; Van Hove, M. A. Phase shift program package, available from http://electron.lbl.gov/software/software.html