The role of molecular t-matrices in LEED theory

María Blanco-Rey* and Pedro de Andrés
Instituto de Ciencia de Materiales (CSIC), Cantoblanco, E-28049 Madrid (SPAIN)
*email: maria.blanco@icmm.csic.es

Georg Held and David A. King
Department of Chemistry, University of Cambridge, Cambridge CB2 1EW, Cambridge (UK)

Within the usual framework of LEED theory [1], we compute the electron scattering inside a molecule via a Dyson-like equation, using free space Green propagators in spherical wave basis [2]. A non-diagonal t-matrix is obtained, containing all the multiple intra-molecular scattering processes. This matrix is particularly useful when studying ordered molecular adsorbates, as it can be easily introduced in any LEED code. The matrix of the rotated or translated molecule can be computed using Wigner matrices or Green propagators respectively. The method is limited by the maximum angular momentum number, because a high number of spherical waves are needed to account for long intra-molecular distances. A direct application of molecular t-matrices to experiment is the description of thermal vibrations that keep the molecule invariant. We explore this possibility in the case of the adsorption of benzene on Ni {111}.

References

[1] J.B. Pendry, "Low-Energy Electron Diffraction", (Academic, 1974)

[2] S. Andersson and J.B. Pendry, J. Phys. C: Solid St. Phys., **13** (1980) 3547

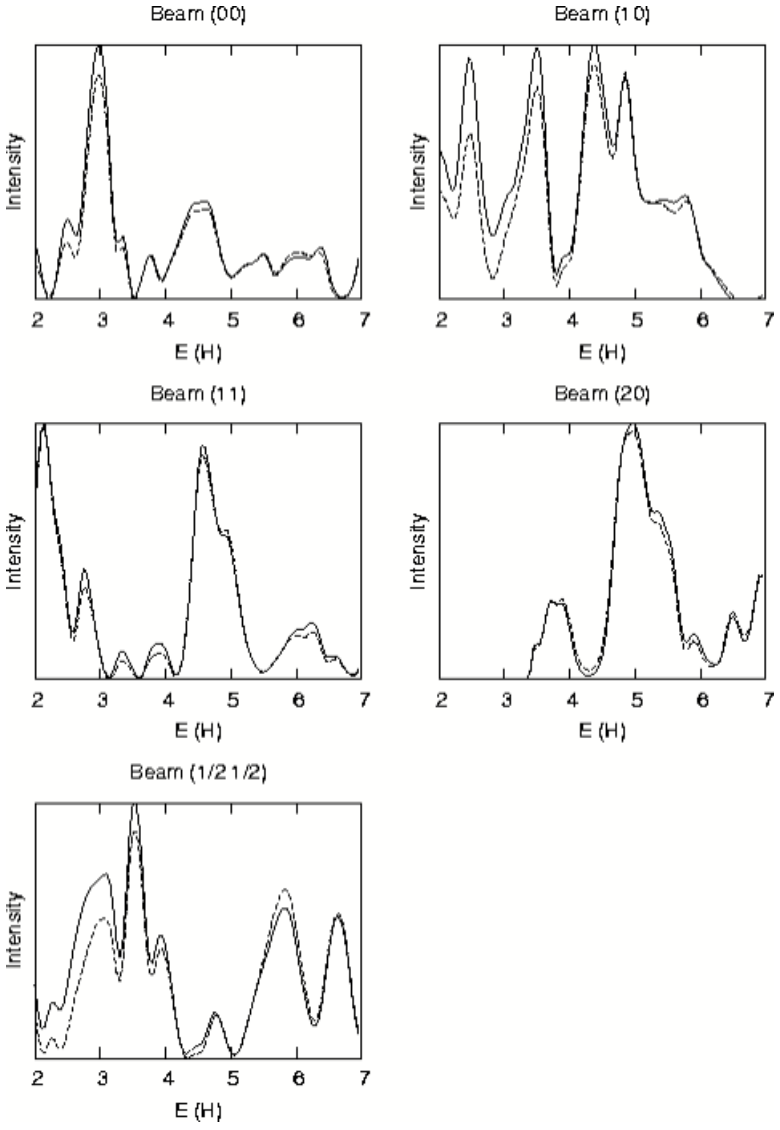

Figure: IV curves for upright CO molecules adsorbed on Cu{100} in top position with c2x2 symmetry. The solid lines correspond to a usual LEED calculation, taking individual atoms, and the dashed lines correspond to the calculation with molecular t-matrices. The maximum angular momentum number is 8 in both calculations. The distance between C and Cu atoms is 1.83 A and 1.2 A between C and O.