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Theoretical study of noble gases diffraction from Ru(0001) using van der Waals DFT-based potentials

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Synopsis This study aims to analyze the role of van der Waals forces in the diffraction process of noble gases from a metal surface. We made use of different vdW implementations to rationalize the effect of dispersion forces on the corrugation of the system, the resulting scattering patterns and on the eventual diffraction results.

Motivated by recent experimental studies about He, Ne and Ar diffraction from a Ru(0001) surface [1], where the last two cases display anticorrugation effects, i.e. corrugation inversion, and by the possibility of using van der Waals (vdW) DFT functionals which allow one to simulate accurately the mentioned experiments, we have studied these systems from a theoretical point of view, aiming to determine the role of vdW interactions on the anticorrugation phenomena observed in the mentioned diffraction processes.

To achieve this task, we built the 3D potential energy surfaces (PESs) based on periodic DFT calculations performed by means of the Vienna ab initio simulation package (VASP) [2].

We tested different vdW functionals during these calculations in order to simulate the dispersion forces. Finally, the diffraction spectra are being computed using both classical and quantum dynamics simulations. Although diffraction is a 'pure' quantum phenomenon and quantum dynamics is, in principle, unavoidable to study our system, a classical analysis based on parallel momentum binning [3] has already been revealed as a very useful tool to mimic and analyze diffraction spectra [4,5].

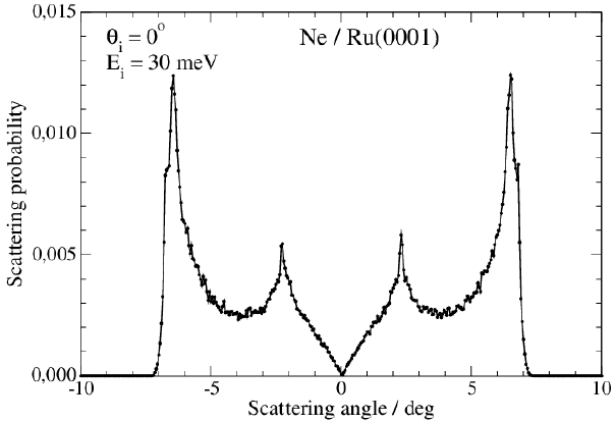

Figure 1. Scattering probability of Ne over Ru(0001) at normal incidence. The scattering distribution presents a classical rainbow, which is proportional to the surface corrugation and will therefore determine the diffraction distribution.

References

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