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He atom scattering from ZnO surfaces: calculation of diffraction peak intensities using the close-coupling approach

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Abstract

Diffraction intensities of a molecular He beam scattered off the clean and water-covered ZnO($10\bar{1}0$) surface have been simulated using a new potential model in conjunction with the close-coupling formalism. The effective corrugation functions for the systems He–ZnO($10\bar{1}0$) and He–H_2O/ZnO($10\bar{1}0$) have been obtained from density functional theory calculations within the Esbjerg–Nørskov approximation. Using these data a potential model is constructed consisting of a corrugated Morse potential at small He–surface distances and a semiempiric attractive part at larger distances. The diffraction patterns obtained from close-coupling calculations agree with the experimental data within about 10%, which opens the possibility to simulate He diffraction from surfaces of any structural complexity and to verify surface and adsorbate structures proposed theoretically by employing this kind of analysis.

(Some figures in this article are in colour only in the electronic version)