Chapter 12
Conclusions about theoretical foundations and simulation of surface structures

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In conclusions, we have discussed the modern theoretical formalisms and numerical tools to simulate the microscopic surface atomic structure and demonstrated their application for main prototypical low-index clean solid surfaces. This aims in explaining, interpreting, and quantifying experimentally determined surface structures, including most complex ones. We also demonstrated the power of the theoretical approaches to predict new surface atomic geometries or complement incomplete experimental structural results. This is the case, for instance, of various technologically important growth processes, where the standard surface-sensitive techniques might not be applied. Although only clean prototypical surfaces were considered in the contribution, the theoretical and computational tools discussed are also directly applicable to the adsorbate-modified surfaces, various interfaces with crystalline solids, and 2D systems such as graphene and graphene-like materials. The above formalisms also allow treating surface defects, roughening or melting transitions, which occur at high temperatures, leading to the loss of 2D translational symmetry.

Despite the remarkable progress of the surface structure simulation formalisms during the last three decades, experimental and technological advances in surface science offer new challenges and open new frontiers for the theorists in even more realistic and accurate simulation in the vast area of surface applications.

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