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Commensurate ground states of monolayers on surfaces ALEXANDRE TKATCHENKO, Universidad Autonoma Metropolitana — We present a procedure for generation of *all* commensurate monolayer-surface structures of a given symmetry, up to a certain number of adsorbate particles (atoms or molecules), N_{ads}, in the unit cell. It is shown that each cell is related to a well-defined sequence of Fourier terms of the single particle-surface potential. Most importantly, the knowledge of Fourier amplitudes alone is sufficient to exactly predict the ground states of commensurate structures in multi-adsorbate unit cells. The impact of the developed theory for theoretical (i.e. DFT simulations) and experimental (LEED studies) determination of commensurate monolayer ground states is briefly discussed. Furthermore, the experimental results for epitaxy of alkali atoms on the Ag(111) surface and iodine on the Pt(111) surface can be described by this approach, in contrast to previous epitaxy theories.

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