Similarities and trends in adsorbate induced reconstructionstructure and stability of FCC iron and cobalt surface carbides

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Thin FCC (100) iron and cobalt carbide films were prepared on Cu(100) to study the connection between their structure, electronic properties and stability. We present the first detailed, real space experimental confirmation of the C-induced clock reconstruction on the FCC(100) surfaces of iron and cobalt. Both Fe and Co surface carbides show p4g (2×2) surface reconstruction with tetracoordinated square planar carbon and pure FCC (100) metal layers underneath. Combining tip-sample distance dependent STM imaging with theoretical calculations we present different imaging modes of Fe₂C. Using a combination of angle-resolved x-ray photoelectron spectroscopy (AR-XPS), Auger electron spectroscopy (AES), low energy electron diffraction (LEED), scanning tunneling microscopy (STM), and theoretical calculations we provide detailed electronic and structural models for Fe₂C and Co₂C p4g (2x2) surface carbides and other 2D Fe₂X interstitial compound systems. In various Fe₂X (X = B, C, N, O) surface compounds moving to the right in the periodic table with increasing electrons the reconstruction becomes less favorable, while iron carbide shows the highest stability.

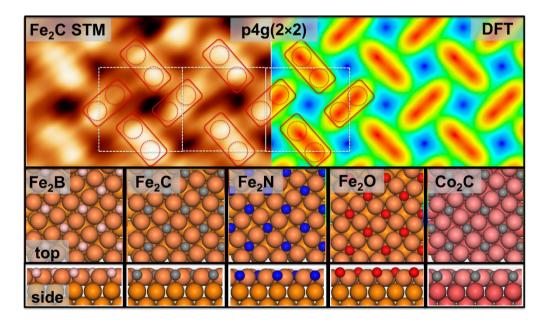


Fig. 1. Upper row - experimental and simulated STM image of Fe₂C surface carbide; second row - calculated surface geometries of Fe₂B, Fe₂C, Fe₂N, Fe₂O and Co₂C slabs, showing the top and side view of the different compounds. All of them follows (near)p4g except Fe₂O.