CHLORINE ATOMIC CHAINS ON Ag(111) SURFACE

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S u m m a r y

The formation of chlorine chain structures on an Ag(111) surface is studied within the Monte-Carlo simulation method. Parameters of the lateral interaction calculated in the framework of density functional theory are used. The chain formation was shown to stem from the indirect interaction between chlorine adatoms owing to Friedel oscillations of the conduction electron concentration emerging when partially charged adatoms are screened. The numerical simulation allowed the formation of the experimentally observed sequence of chlorine structures on the Ag(111) surface to be explained. In particular, the mechanism of transformation from the chain structure into the hexagonal $(\sqrt{3} \times \sqrt{3})\mathrm{R}30^\circ$ one as the coverage increases to $\theta = 0.33$ has been elucidated.