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Atomic and Electronic Processes During the Formation of an Ionic NaCl Monolayer on Si(100)¹ DENG-SUNG LIN, CHAN-YUEN CHANG, HONG-DAO LI, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan, SHIOW-FON TSAY, Department of Physics, National Sun Yat Sen University, Kaohsiung, Taiwan, CHAN-YUEN CHANG, HONG-DAO LI, DENG-SUNG LIN TEAM, SHIOW-FON TSAY COLLABORATION — An atomic layer of stoichiometric NaCl was formed on a covalent Si(100) surface after two successive halfreactions at room temperature. The first half-reaction due to Cl₂ exposure generates a square array of Cl adatoms with a distance close to that in a NaCl(100) surface plane. By utilizing scanning tunneling microscopy, core-level photoemission spectroscopy and ab initio density functional theory calculations, it was found that progressive deposition of Na in the second-half reaction results in surface-supported Na₃Cl clusters, one dimensional cluster chains and (2x2) patches, and eventually turns the Cl-adlayer into a single-terrace, wavy NaCl layer at one monolayer Na coverage. The grown NaCl monolayer rolls over atomic steps like a carpet and covers the entire surface. The atomic and electronic structure of the topmost Si layer underneath the NaCl layer resembles that of the initial silicon surface layer with buckled dimers. Results of the comprehensive investigation together suggest that an ionic NaCl monolayer is very weakly bonded to the covalent substrate and appears nearly free standing.

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