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Self-Assembly of Glycine on Cu (001): The tale of Temperature and Polarity LIFANG XU, Institute of Physics, Chinese Academy of Sciences, JING XU, Department of Physics, Renmin University of China, ZHESHUAI LIN, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, SHENG MENG, ENGE WANG, Institute of Physics, Chinese Academy of Sciences — Glycine on Cu(001) is used as an example to illustrate the critical role of molecular polarity and finite temperature effect in self-assembly of bio-molecules at a metal surface. A unified picture for glycine self-assembly on Cu(001) is derived based on full polarity compensation considerations. Temperature plays a non-trivial role: the ground-state structure at 0 K is absent at room temperature, where intermolecular hydrogen bonding overweighs competing molecule-substrate interactions. The unique p(24) structure predicted as the most stable structure was confirmed by ab initio molecular dynamics simulations, whose scanning tunneling microscopy images and anisotropic free-electron-like dispersion are in excellent agreement with experiments. Moreover, the rich self-assembling patterns including the heterochiral and homochiral phases, and their interrelationships are entirely governed by the same mechanism.

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