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Atomistic Processes in Self-Assembly of Millimeter-Sized Conducting Graphenne on Cu(111)[1] PING CUI, HONGBIN ZHU, JIN-HO CHOI, QIANG ZHANG, XIAOXIA LI, FANGFEI MING, ZHENYU LI, JINLONG YANG, CHANGGAN ZENG, ZHENYU ZHANG, University of Science and Technology of China — In a latest study, we have fabricated a new two-dimensional material which we call graphenne, consisting of perfectly ordered N dopants in a graphene matrix. Due to the doped electrons and the ordered nature of the N dopants, the newly discovered graphenne is a highly conducting crystal possessing superb electronic properties. Using density functional theory calculations, here we investigate the atomistic processes in the fabrication of graphenne on Cu(111) using molecular precursors, and reveal the elegant concerted roles played by the London dispersion, chemical, and screened Coulomb repulsive forces in enhancing molecule-substrate binding, facilitating easy detachment of the terminating atoms, and dictating the overall orientation of the remaining radicals, respectively. Furthermore, in contrast to graphene growth, the ordered N atoms anchor the selection of a single orientation relative to the substrate, effectively suppressing the creation of orientational disorders such as grain boundaries as the islands coalesce to form graphenne samples as large as the millimeter-sized Cu(111) substrate. These findings are directly compared with experimental observations.

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