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Hexagonal motifs on the Ir(100) surface reconstructions from a first-principles study WAN-SHENG SU, National Center for High-Performance Computing, Tainan 741, Taiwan, FENG-CHUAN CHUANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan, KEN-MING LIN, TSAN-CHUEN LEUNG, Department of Physics, National Chung Cheng University, Chia-Yi 621, Taiwan — The hexagonal motifs of the Ir(100) surface overlayer are examined by using first-principles calculations. The studied hexagonal motifs are formed on the Ir(100) surface overlayer with (5x1), (8x1), (12x1), and (14x1) periodicities. Our results showed that the unstrained (5x1) phase is the most stable phase, which is consistent with not only previous theoretical calculations but also experimental findings. Further analysis on the strain-induced phase transition among various hexagonal reconstructions is presented. Such a phenomenon can be further qualitatively elucidated by analyzing the computed average standard deviation of angles.

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