Molecular Dynamics Study of Physisorbed Xenon on Ai(1 1 0)

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Abstract

The adsorption of Xe on the (1 10) face of an AI substrate is investigated by means of molecular dynamics. A thermodynamic transformation at constant temperature is studied as a function of the Lennard-Jones potential range parameter gxe_At, for several sizes of the Xe island adsorbed on AI. This way a critical value of cxe_AI, for which the island undergoes a commensurate-incommensurate transition, is identified. The implications of our results are discussed in the context of experimental interpretation and comnared with nublished Monte Carlo work on this system.