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Dimer Adsorption on (100) Terraces With First- and Second-Neighbor Interactions[1] ALAIN PHARES, Villanova University, MARCELO PASINETTI, Universidad Nacional de San Luis, Argentina, DAVID GRUMBINE, JR., St. Vincent College, FRANCIS WUNDERLICH, Villanova University — Adsorbed particles that binds to two nearest-neighbor sites, such as CO/Ni(100), are simulated as dimers covering infinitely long (100)-terraces of finite width M, with first- and second-neighbor interaction energies, V and W. The set {coverage, number of first-neighbors per site, number of second-neighbors per sites}, and the entropy characterize the adsorption system. For attractive first-neighbors ($V > 0$) there are two series of phase diagrams, for M even and odd, which coincide in the infinite-M limit, with one non-trivial phase {1/2, 1/4, 0} for $W/V < -1/2$. For repulsive first-neighbors, the phase diagrams are obtained for $M \leq 7$. In the infinite-M limit, the non-trivial phases are, {1/3, 0, 0}, {1/2, 1/4, 0}, {1/2, 0, 1/2}, and {2/3, 1/3, 1}. Past computations, which neglected second-neighbor interactions and considered V<0, found only two phases {1/2, 0, 1/2}, and {2/3, 1/3, 1}. Here, these results are recovered, and in the infinite-M limit, Monte Carlo simulation and finite-size scaling are used to obtain the heat capacity and the critical temperature of the order-disorder transitions as a function of W/V. [1]Work supported by NSF and the PSC (AP and DG), and by CONICET and the Fulbright Foundation(MP).

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