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Binding site H3 to T4 occupation switching and the Pb/Si(111)"Devil's Staircase" phase diagram<sup>1</sup> V. YEH, M. YAKES, M. HUPALO, M.C. TRINGIDES, Ames Laboratory-Iowa State University, Z. CHVOJ, Czech Academy of Science — With SPA-LEED and STM it has been observed that there is a switching occupation from only H3 sites to H3 and T4 sites within the unit cell of the DS ("Devil's Staircase") (n,m) linear phases at the (1,1) phase or theta=1.25ML. This is observed from the doubling of the linear phase period and the "flipping" of the triangle diffraction pattern. The transition temperature from linear to HIC shows a minimum at  $\sim 120$ K for the (1,1) phase and follows a U-shaped curved in the whole DS range 6/5ML < theta < 4/3. This unusual dependence (instead of the monotonic decrease of the transition temperature expected for repulsive interactions) indicates the presence of other interactions in the system which can originate from the binding site switching. A statistical mechanical model that includes these two interactions is analyzed and accounts semi-quantitatively for the U-shaped curve and the phase diagram topology. However, a complete treatment should also include the comparison with the free energy of the HIC phases since the linear phases transform to these phases at higher temperatures. The binding site H3 to T4 switching is also relevant to theoretical predictions for the ordered phases in Ba(3x2) grown on stepped Si(111) due to the presence of similar long range interactions.

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