Adsorption on Nanotubes With Repulsive First Neighbors

ALAIN PHARES, Villanova University, DAVID GRUMBINE, St. Vincent College, FRANCIS WUNDERLICH, Villanova University — We consider adsorption on nanotube lattices with zigzag triangular geometry. In Langmuir, Vol. 24, pp. 11722-11727 (2008), we studied such adsorptions with first- and second-neighbor interactions and attractive first-neighbors. The nanotube energy phase diagram is independent of \( M \), the number of atoms in the nanotube circumference, and holds for infinite \( M \), reproducing the infinite width limit of a triangular terrace [Langmuir, Vol. 24, pp. 124-134 (2008)]. Here, we consider repulsive first-neighbors. The phase characteristics, \( \{ \theta_0, \theta, \beta \} \), are the coverage, and the numbers per site of first and second neighbors, respectively. Particle-hole symmetry holds for all nanotube diameters and the energy phase diagram is \( M \) dependent. In the infinite-\( M \) limit, the non-trivial phases with their complements are: \( \{1/4, 0, 0\} \), or \( (2 \times 2) \), and \( \{3/4, 3/2, 3/2\} \); \( \{1/3, 1/3, 0\} \), or \( (3 \times 1) \), and \( \{2/3, 4/3, 1\} \); \( \{1/3, 0, 1\} \), or \( (\sqrt{3} \times \sqrt{3}) \) \( R30^\circ \), and \( \{2/3, 1, 2\} \); and \( \{1/2, 1/2, 1/2\} \), which is its own complement. This infinite-\( M \) limit should be the same as the infinite width limit of a triangular terrace. We found that we had missed the \( \{2/3, 4/3, 1\} \)-phase in Langmuir, Vol. 23, pp. 1928-1936 (2007).

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