Adsorption on Nanotubes With Repulsive First Neighbors[1]

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 (2×2), and $\{3/4, 3/2, 3/2\}$; $\{1/3, 1/3, 0\}$, or (3×1), and $\{2/3, 4/3, 1\}$; $\{1/3, 0, 1\}$, or $(\sqrt{3} \times \sqrt{3})$ R30°, 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).

Alain Phares
Villanova University

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