Abstract Submitted for the MAR14 Meeting of The American Physical Society

Low Temperature Energy Phase Diagrams of Dimer Adsorption on Square Nanotubes with Repulsive First-Neighbor Interactions¹ ALAIN PHARES, Villanova University, DAVID GRUMBINE, JR, St. Vincent College — We consider dimer adsorption on infinitely long square nanotube surfaces with increasing diameter which, when keeping the lattice constant fixed, corresponds to an increasing number M of atomic sites in the normal section of the nanotube. We present the low temperature energy phase diagram of the system which is generated assuming repulsive first-neighbors and arbitrary second-neighbor interactions. The occupational characteristics of the system are the coverage, θ_0 , and the numbers of first- and second-neighbors per sites, θ and β . Crystallization patterns (phases) occur at values of the set { θ_0 , θ , β } given explicitly as functions of M. The regions of the phase diagram in which the phases are found have been determined for any M, allowing an exact extrapolation to the infinite M limit.

¹Work supported by the National Institute for Computational Sciences, Grant # TG-CHE050014.

Alain Phares Villanova University

Date submitted: 15 Nov 2013

Electronic form version 1.4