Abstract Submitted
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Co-adsorption of n Monomer Species on Terraces and Nanotubes[1] ALAIN PHARES, Villanova University — We consider the partition function, Z, of the system of n monomer species adsorbed on a terrace or a nanotube of arbitrary periodic lattice geometry, Latomic sites in length, and M' sites in the width of the terrace or in the normal cross-section of the nanotube. Z is related to the eigenvalues of a real and non-negative matrix (**T** matrix) of rank $(n+1)^M$, where M is an integer multiple of M'. In the infinite-L limit, we also prove that Z is the largest eigenvalue of the **T**-matrix, raised to the power $1/M$. Because the rank of this matrix increases exponentially with M, we develop a technique for its recursive construction applicable to any lattice geometry, which is easily programmed and efficiently adaptable for supercomputing and multiparallel processing. As examples, we consider the co-adsorption on square, equilateral triangular, and honeycomb surfaces. This general formulation can now be applied to model a whole new set of experiments involving the coadsorption of two or more monomer species, on terrace or nanotube surfaces with various periodic lattice structures.

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