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Adsorption thermodynamics of a lattice–gas model with non-additive lateral interactions on triangular and honeycomb lattices

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ABSTRACT

Adsorption thermodynamics of a lattice–gas model with non-additive interactions between adsorbed particles for triangular and honeycomb lattices is discussed in the present study. The model used here assumes that the energy which links a certain atom with any of its nearest-neighbors strongly depends on the state of occupancy in the first coordination sphere of that adatom. By means of Monte Carlo simulations in the grand canonical ensemble the adsorption isotherms and isothermal susceptibility (or equivalently the mean square density fluctuations of adparticles) were calculated and their striking behavior was analyzed and discussed in terms of the low temperature phases formed in the system.

1. Introduction

The interest in the study of adsorption process on solid surfaces has been enhanced in the past decades. This interest is based in the essential role that this phenomenon plays in many experimental situations, such as heterogeneous catalysis, oxidation, lubrication, coating, melting, roughening, crystal and film growth and gas separation, just to name a few [1–5].

In several contributions, the physisorbed monolayers at solid surfaces are described in terms of the well-known lattice–gas (LG) model [1–6]. This description is expected to retain majority of the properties of the system under study avoiding the difficulties of an analytical treatment of typical many-body problems. In addition, the LG models allow a deeper understanding of a variety of ordering phenomena and a simple practical implementation through numerical techniques. However, the description of more complex systems by means of LG models could not be enough to consider the complete variety of interactions present in a given problem. As a simplification of the problem, it is a traditional assumption to assign purely additive interactions to the adsorbate–adsorbate coupling which is accepted as a crude approximation only.

For several experimental arrangements the behavior of the thermodynamic quantities and the phase diagram of the system differ significantly from those predicted by using a LG model with additive interactions [7]. Thus, it is concluded that experimentally observed phase diagrams can be obtained using hamiltonians with terms accounting for more complex ad–ad interactions. Surface restructuring is another example of a system where more complex ad–ad interactions take place [8–14]. In fact, the deviation of an additive behavior appears to be especially significant in the case of chemisorption where the valence electrons are either concentrated in forming a single bond between two isolated atoms, or shared among all neighbors which occasionally occupy sites in the first coordination shell of the central atom. In fact, non-additive ad–ad interactions have been observed in several experimental systems [15].

The consequences of considering non-pairwise (non-additive) interactions in the adsorption thermodynamics have been studied for a long time by means of mean field approximation (MFA) [16–18] and the quasichemical approach (QCA) [19]. On the other hand, in Ref. [20], a Monte Carlo study of adsorption of monomers with non-additive interactions on square

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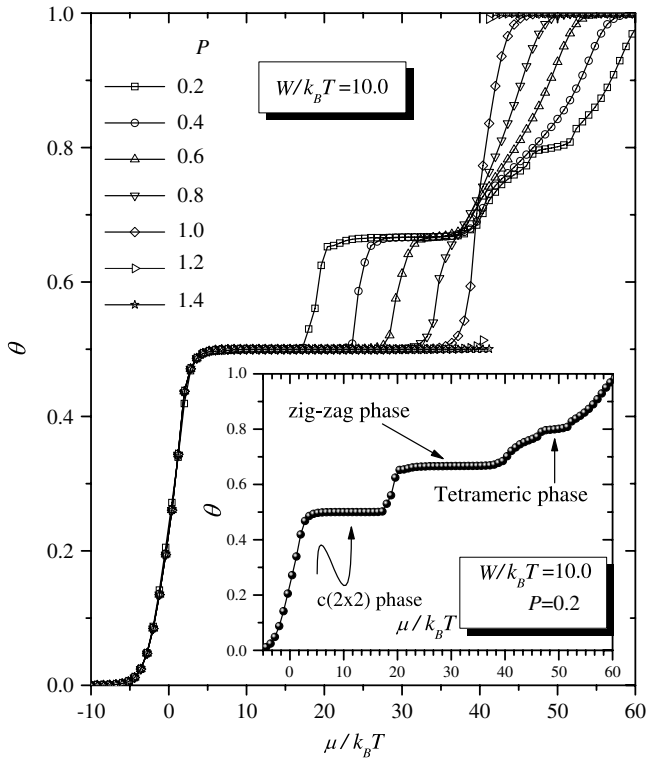

Fig. 1. Adsorption isotherms for a fixed temperature and different values of the non-additivity parameter, P, as indicated for square lattice. The inset shows the adsorption isotherm for $P = 0.2$ where the plateaus are clearly identified and associated to the different low temperature ordered phases.

lattice has been presented. In particular, the thermodynamics for repulsively interacting particles has been considered. Thus, adsorption isotherms, isothermal susceptibility (or equivalently the mean square density fluctuations of adparticles) were calculated by means of Monte Carlo simulations in the grand canonical ensemble. It is possible to summarize the results of Ref. [20] by considering two cases. If the non-additivity tends to weaken the $c(2 \times 2)$ ordered phase (as compared to the additive case), it is possible to distinguish the presence of different low temperature ordered phases depending on the surface coverage. In fact, the evidence of (a) very wide plateaus in the adsorption isotherms; (b) weak peaks in the thermodynamic factor (revealing the entrance in the ordered phase); (c) steps in the isosteric heat; allow us to conclude the existence of different low temperature ordered phases. It is interesting to mention that some of them are formed by structures of adatoms ordered like "dimer" or "tetrameric" phases which are observed in experiments [15]. For cases where the non-additivity tends to reinforce the $c(2 \times 2)$ phase it exists evidence of the presence of a continuous phase transition from the $c(2 \times 2)$ structure to disorder around to half coverage. However, the most interesting result is the evidence of a first order phase transition in the vicinity of $\theta \approx 0.72$. A complete panorama is given in Fig. 1 where the adsorption isotherms are shown for different degrees of non-additivity and a fixed low temperature (low temperature should be understood as lower than a critical temperature). The present contribution goes one step further by describing the behavior of the same model as in Ref. [20] but now in different geometry: triangular and honeycomb lattices.

The influence of the phase transition due to additive interactions on the adsorption process has been studied by means of theoretical, experimental and numerical methods. It is well known that the LG model is equivalent to the Ising spin model in an external magnetic field. Taking into account that a occupied (vacant) site can be represented by an spin up (down) is fully equivalent to discuss the problem in terms of either spin representation or LG terminology. In order to explain the phase transition in the case of additive interactions we prefer to use the spin representation because of its apparent symmetry with respect to the external magnetic field. However, we shall refer to lattice–gas terminology in most of the paper or where it seems to be more transparent. For ferromagnetic interactions there is a critical point at $J/k_BT = \frac{1}{4} \ln 3 \approx 0.2747$ (where J is the interaction parameter). This point corresponds to the second order phase transition between disordered and ferromagnetically ordered phases. For antiferromagnetic interactions, the critical point is absent for all finite T due to the huge degeneracy of the ground state. It is easy to show from simple energy arguments that for (a) antiferromagnetic interactions and (b) strong magnetic field the ground state is ferromagnetically ordered: all spins are up for $h > 0$ and down for $h < 0$ [being $h = (\mu + 3J)/2k_BT$ and μ the chemical potential]. Antiferromagnetic ordering is possible for finite temperatures if the magnetic field is weak. In order to explain the antiferromagnetic ordering we recall that a triangular lattice can be seen as a system composed of three equivalent triangular sublattices. There are two antiferromagnetically ordered phases: one for $h > 0$ and one for $h < 0$. Both antiferromagnetically ordered phases correspond to the threefold

degenerate ground state with all spins of any two sublattices aligned along the direction of the external magnetic field h and all spins of the third sublattice aligned in the opposite direction $\uparrow\uparrow\downarrow$, $\uparrow\downarrow\uparrow$, $\downarrow\uparrow\uparrow$ ($h > 0$) and $\downarrow\downarrow\uparrow$, $\downarrow\uparrow\downarrow$, $\uparrow\downarrow\downarrow$ ($h < 0$). The ferromagnetically ordered structures will be denoted as $\downarrow\downarrow\downarrow$ for $h < 0$ and $\uparrow\uparrow\uparrow$ for $h > 0$.

In the case of honeycomb lattices, a phase transition exists at coverage 1/2, for repulsive and additive interactions. Strong lateral interactions cause ferromagnetic ($J > 0$) or antiferromagnetic ($J < 0$) phase transitions. The exact critical value of the interaction parameter in the absence of an external magnetic field is equal to $J/k_BT = \pm 0.5 \ln(2 + \sqrt{3}) \approx 0.658478$ [21].

As a natural extension of previous studies, we present in this paper the adsorption of monomers with non-additive and repulsive interactions on two very important lattices in the description of adsorption: triangular and honeycomb lattices.

The paper is organized as follows. In Section 2, we briefly recall the lattice–gas model which includes the non-additive interactions. In Section 3 we summarize the Monte Carlo technique in the grand canonical ensemble. In Section 4, results are presented and discussed for the adsorption thermodynamics and we finish in Section 5 with the conclusions and future perspectives.

2. The theoretical model

We shall consider an idealized solid surface of honeycomb and triangular symmetry. The minima of the potential energy on such surfaces form a homogeneous two-dimensional array with constant a where each adsorbed particle has a coordination number $z = 3\,(6)$ for honeycomb (triangular) array. Each adsorption site can be occupied only by one particle (multiple occupation of sites is excluded). Then, the adsorbed phase is characterized by the hamiltonian

$$H = -\varepsilon \sum_{i=1}^{M} c_i - \sum_{i \neq j}^{M} W_{ij} c_i c_j \tag{1}$$

where i and j denote the adsorption sites, the local occupation variable c_i is 0 (1) if the adsorption site is empty (filled) and the second sum is over the nearest-neighbor sites. ε reflects the interactions between the substrate and the adatoms, which is independent of the temperature and coverage, and can be considered equal to zero without losing generality. The adsorbate–adsorbate interaction, W_{ij} is assumed to depend on the occupation state of the surrounding of a given site i. Following the line of thinking presented in a previous work, Ref. [20], we consider the simplest model of non-additive interaction energies. It is assumed that (i) W_{ij} has different possible values, $\{W_1, W_2, \ldots, W_z\}$ depending on how many first neighbors are actually present in the vicinity of a given atom, (ii) the energy interaction between a given atom and any of its nearest-neighbors varies linearly with the number of them and (iii) W_m varies linearly with m and $W_z = W$. Following Ref. [18] the parameter of non-additivity, $P = W_1/W_z$ is introduced as a measure for the stronger to the weakest bond possible in each system:

$$\frac{W_m}{W} = \frac{Pz - 1}{z - 1} - m\frac{P - 1}{z - 1}. \tag{2}$$

This situation has been tackled by MFA [16] and by the configuration-counting procedure of the well-known QCA [17]. However, the analysis given in the cited papers has been restricted to square lattices mainly including attractive interactions. The discussion presented in the present paper covers the entire range of interactions, temperatures and coverage for triangular and honeycomb lattices.

3. Monte Carlo simulations of adsorption–desorption processes in the grand canonical ensemble

The adsorption–desorption process on an adsorptive surface is considered by putting in contact $M = L \times L$ adsorption sites with an ideal gas phase of particles at temperature T [22,23]. The particles are characterized by their chemical potential μ. The surface as well as the adsorbent are inert upon adsorption. In the grand-canonical ensemble, μ, T and the generalized volume V of the physical system are the thermodynamics parameters. We use Metropolis scheme [24] to satisfy the principle of detailed balance.

The interested reader will find a detailed analysis of the algorithm in Ref. [20]. In order to inform the Monte Carlo parameters of the simulations we establish that one Monte Carlo step (MCS) corresponds to L^2 attempts of changing the state of the system. The first $m' \approx 10^6$ Monte Carlo steps (MCS) of each run were discarded for allowing to reach the equilibrium state and the next $m \approx 10^6$ MCS were used to compute averages.Then the thermodynamic quantities of interest, such as mean coverage, θ, and mean adsorption energy per site, u, are obtained by simple averaging:

$$\theta = \frac{1}{M}\sum_{i}^{M}\langle c_i \rangle; \qquad u = \frac{1}{M}\langle H \rangle. \tag{3}$$

The thermodynamic factor is a quantity of interest and it can be obtained in one of its two equivalent forms:

$$T_f = \left(\frac{\partial \beta\mu}{\partial \ln\theta}\right) = \left[\frac{\langle (\delta N)^2 \rangle}{\langle N \rangle}\right]^{-1} \tag{4}$$

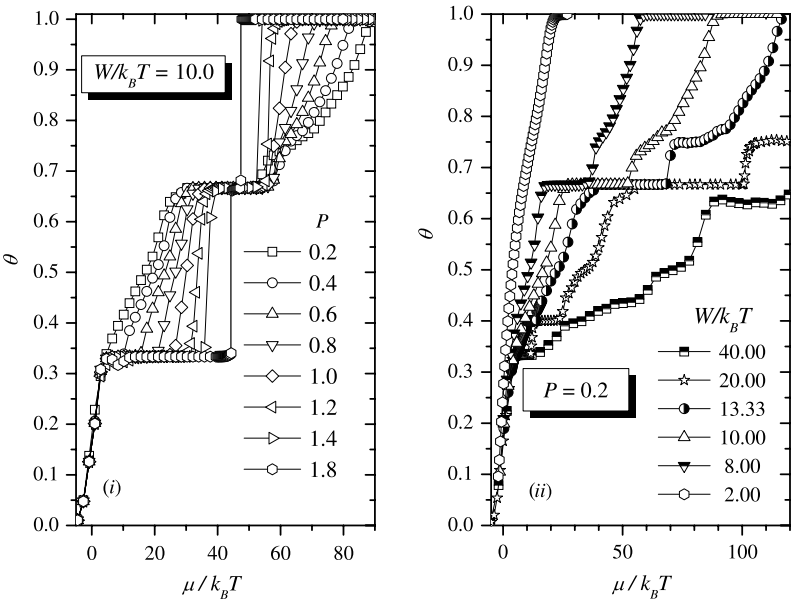

Fig. 2. Adsorption isotherms for triangular lattice (surface coverage θ versus the normalized chemical potential μ/k_BT) for (i) a fixed temperature and different values of the non-additivity parameter, P, as indicated and (ii) for $P = 0.2$ and several values of temperature expressed in units of W/k_BT as indicated.

either via the differentiation of adsorption isotherms obtained in the grand canonical ensemble [25] or via the normalized mean square fluctuations $\frac{\langle(\delta N)^2\rangle}{\langle N\rangle}$ obtained in canonical ensemble. Thus, the thermodynamic factor can be related with the isothermal susceptibility, χ_T by:

$$T_f = \theta\left(\frac{\partial^2 F}{\partial\mu^2}\right)^{-1} = \frac{\theta}{\chi_T} \tag{5}$$

where F is the free energy of the system. The thermodynamic factor is an important quantity because it is needed for the calculation of the chemical diffusion coefficient [26–28].

4. Results and discussions

We shall start by discussing the behavior of adsorption isotherms in a triangular lattice with non-additive nearest-neighbor repulsive interactions between adparticles. By using lattices sizes larger than $L = 256$ we have verified that finite size effects are negligible. In Fig. 2(i), adsorption isotherms for a low temperature case $W/k_BT = 10.0$ (low temperature should be understood as lower than the critical temperature) and several values of the non-additivity parameter, P are shown. In this figure, it is possible to clearly distinguish two plateaus at definite coverages $\theta = 1/3$ and $\theta = 2/3$. These plateaus are an indication of the presence of a order–disorder phase transition. The low-temperature ordered phases are $\sqrt{3}\times\sqrt{3}$, and $(\sqrt{3}\times\sqrt{3})^*$, respectively, which have been also reported in additive systems [21]. Two regimes of non-additivity can be established, (a) for $P < 1.0$ and the second one (b) for $P > 1.0$. In the former, the first (second) plateaus at $\theta = 1/3$ ($\theta = 2/3$) is less (more) wide upon decreasing P. By the contrary, a totally different situation can be described as $P > 1.0$: the first (second) plateaus at $\theta = 1/3$ ($\theta = 2/3$) is more (less) wide.The adsorption isotherms behave in a different way for limit values of P: the ordered phase $\sqrt{3}\times\sqrt{3}$ [$(\sqrt{3}\times\sqrt{3})^*$] disappears at $P = 0.2$ [$P = 2.0$] how it is also shown in Fig. 2(i).

Let us consider first the regime (a). Fig. 2(ii) shows the isotherm for the situation $P = 0.2$ and several values of temperature in term of W/k_BT. At high enough temperatures the isotherms recover the Langmuir case (LG without lateral interactions). At low temperature we can identify four new plateaus. In addition to the previously identified phases $\sqrt{3}\times\sqrt{3}$, and $(\sqrt{3}\times\sqrt{3})^*$, it is possible to determine other new LG ordered phases which are much more evident at very low temperature. Fig. 3(i) shows the isotherm for $P = 0.2$ and $W/k_BT = 20.0$ where the new plateaus appear at coverage $\theta = 0.40$, 0.50, 0.75 and 0.86, respectively. In order to clarify the situation we have labeled each plateau with a letter in rising order of appearance from (a) to (f). The ordered phase is separated from the disorder state by an order–disorder phase transition occurring at a finite critical temperature. An indication of the presence of such transition phases is the behavior of the thermodynamic factor. The coverage dependence of the thermodynamic factor is shown in Fig. 3(ii), for the case reported in 3 (i). The fluctuations exhibit six maxima at the coverage where the ordered phases are established in complete agreement with each plateau of the isotherm. The labels are indicated with the same criterion that in the isotherm. The

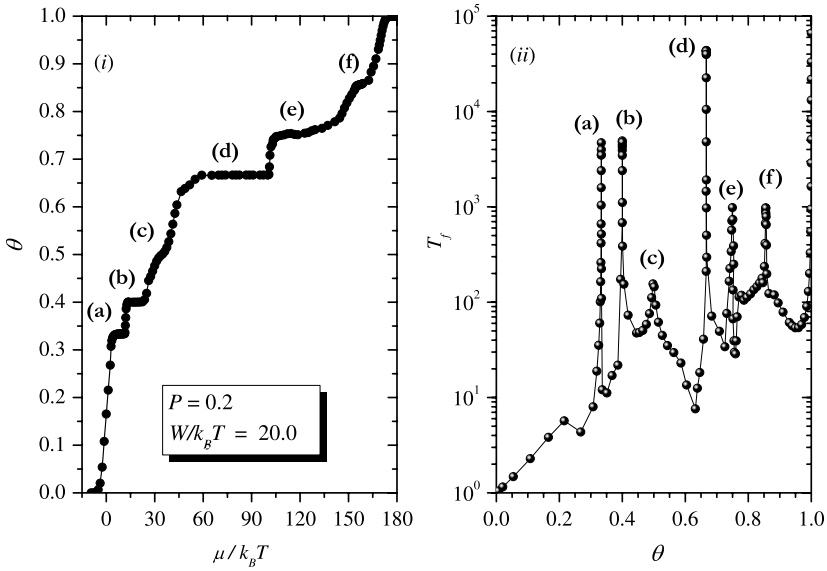

Fig. 3. (i) Adsorption Isotherm (triangular lattice), for $P = 0.2$ and $W/k_BT = 20.0$, where the plateaus are clearly identified. We have labeled each plateau by a letter in rising order of appearance from (a) to (f). (ii) Thermodynamics factor versus coverage for the same condition (i). One can see how a narrow maximum appears at each coverage where the phases are established (the critical coverage are 1/3, 0.40, 0.50, 2/3, 0.75 and 0.86, respectively).

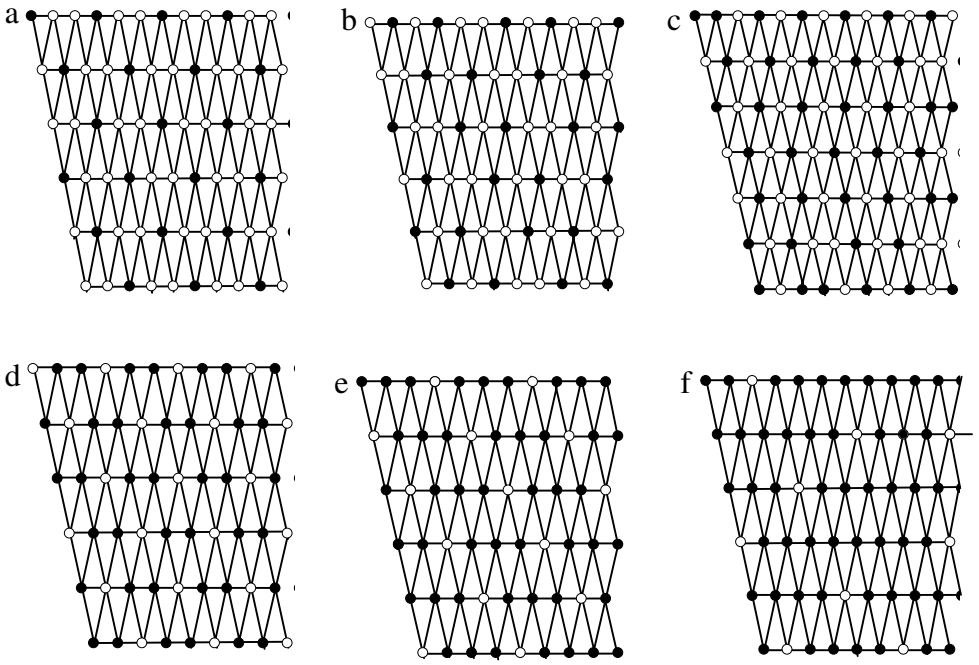

Fig. 4. Typical snapshot of the low temperature ordered phases (triangular lattice). The ordered phases are plotted at: (a) $\theta = 1/3$, (b) $\theta = 0.4$, (c) $\theta = 0.5$, (d) $\theta = 2/3$, (e) $\theta = 0.75$ and (f) $\theta = 0.86$.

fluctuations decrease when θ deviates from the values where the phases are established. The dependence T_f has a large and a narrow maximum at low temperature but remains analytical. To complete the discussion, in Fig. 4 we show snapshots of the corresponding low temperature phases which have been labeled in agreement with Fig. 3. Fig. 4(a) corresponds to $\sqrt{3} \times \sqrt{3}$ phase where each adatom does not have any occupied nearest-neighbor sites. In the case of Fig. 4(b) each adatom presents only one occupied site in its environment; and so on.

Fig. 5 shows the adsorption isotherms for a typical case with $P > 1.0$ [$P = 1.6$, regime (b)] and different values of temperature as indicated. Notice that the limiting case for enough high temperature is recovered. Below T_c, the adsorption isotherms exhibit discontinuities, i.e. two jumps of the surface coverage, (i) from the $\sqrt{3} \times \sqrt{3}$ phase to the $(\sqrt{3} \times \sqrt{3})^*$ one

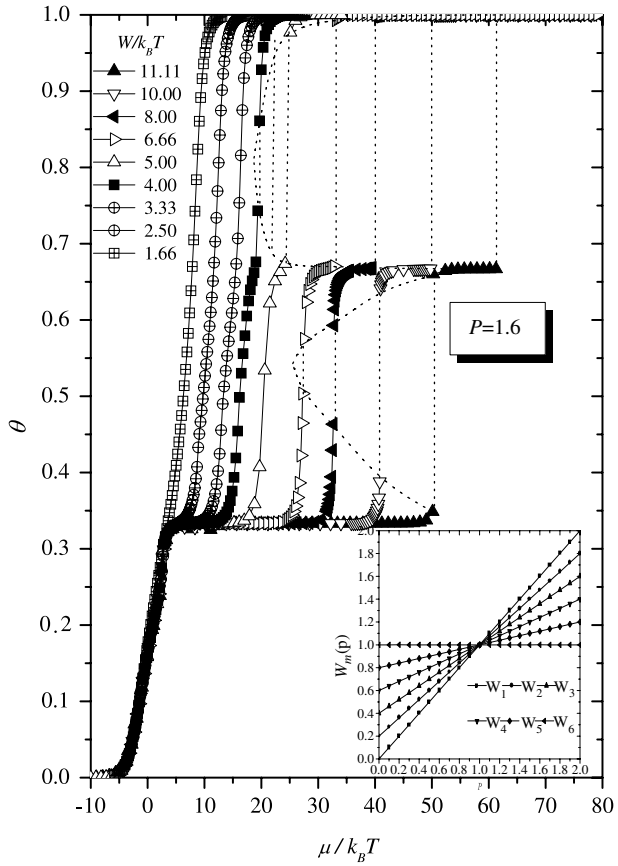

Fig. 5. Adsorption isotherms (triangular lattice) for $P = 1.6$ and different values of temperature expressed in units of W/k_BT. The dashed lines denote the coexistence area and they are shown only as a guide to the eyes.

and (ii) from $(\sqrt{3} \times \sqrt{3})^*$ until filling the lattice. The critical point corresponding to the first jump in the isotherm appears at $\theta_c = 0.542$ and the second one at $\theta_c = 0.80$. This behavior can be understood under considering $W_m(P)$ as shown in the inset of Fig. 5. One can observe that $W_z = 6 < W_i\,(i = 1, \ldots, 5)$, for values of non-additivity larger than one. The system prefers to condensate from $\theta = 1/3\,(2/3)$ to $\theta = 2/3\,(1)$ because any sequential filling smaller than $\theta = 2/3\,(1)$ has a bigger energy than the energy at coverage $\theta = 2/3\,(1)$. When $P > 2.0$ the phase $(\sqrt{3} \times \sqrt{3})^*$ disappears and the system condenses from $\theta = 1/3$ to $\theta = 1$ due to energetic requirements.

Fig. 6(i) shows the energy per site, u, versus coverage for several values of P, and $W/k_BT = 10.0$. Notice how the energy per site changes the slope at the coverage where new phases are established. In the regime $0 < \theta \leq 1/3$ the particles do not interact with each other and $u = 0$ until the $\sqrt{3} \times \sqrt{3}$ phase is formed. Upon increasing the surface coverage each incoming particle interacts with others. Thus, for each formed phase, a new monomer added onto the surface contributes to increase linearly the energy until filling the lattice. In order to clarify this situation, in Fig. 6(ii) the energy per site for $P = 0.2$ and $W/k_BT = 20.0$ is presented. Here, the inset [Fig. 6(iii)] shows a zoom of the energy per site in the coverage range where phases (a), (b) and (c) are present. In fact, one can identify three changes of slope in this interval. For larger values of coverage the slope of the curve changes three times in agreement with phases (d), (e) and (f). For $0.7 < P \leq 1.0$ the only phases that persist are $\sqrt{3} \times \sqrt{3}$ and $(\sqrt{3} \times \sqrt{3})^*$. Then, there are only two changes of slope, as expected. For $P > 1.0$ the energy per site behaves as in a first order transition in agreement with previous results.

We shall discuss now the adsorption of particles with non-additive interactions in a honeycomb lattice. Thus, Fig. 7(i) shows the adsorption isotherms for several values of P and a fixed temperature below the critical one. In a similar way to the case discussed before, two regimes can be distinguished: (a) $P \leq 1.0$ and (b) $P > 1.0$. However it is important to notice that in both regimes a broad plateau appears at coverage $\theta = 1/2$. For regime (a) [(b)], it can be observed how the plateaus at $\theta = 1/2$ become less [more] wide upon decreasing [increasing] P from $P = 1.0$. In the inset of Fig. 7(i) three different plateaus are shown at $\theta = 0.5$, $\theta = 0.625$, and $\theta = 0.75$ for regime (a) and $P = 0.2$. We have labeled each plateau by a letter in rising order of appearance from (a) to (c), respectively. The adsorption isotherms for $P = 0.2$ and several values of temperature plotted in Fig. 7(ii) make more evident the described situation.

In Fig. 8 the thermodynamic factor for the case $P = 0.2$ is shown and the corresponding low temperature phases are schematically presented in the inset. Notice that each maximum corresponds with the coverage value where the phases are

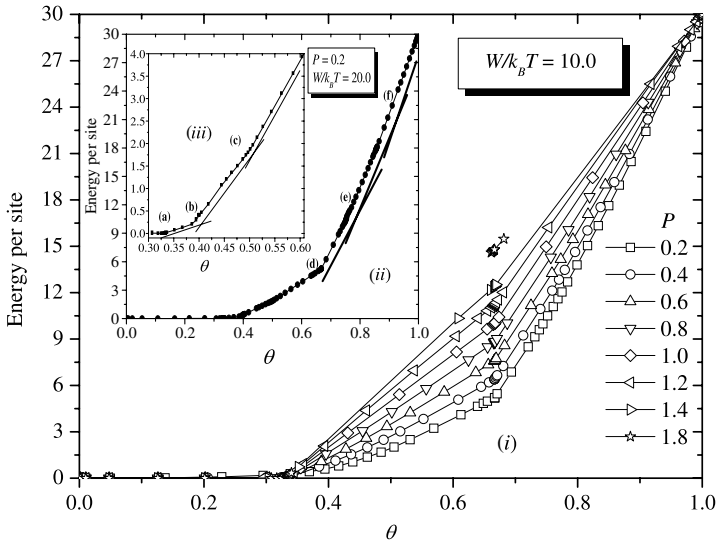

Fig. 6. Energy per site, u, versus lattice coverage (triangular lattice) for (i) a fixed value of W/k_BT and different values of the non-additivity parameter, P as indicated. (ii) u, versus θ for $P = 0.2$ and a fixed value of W/k_BT while (iii) shows a zoom of the same curve for a small range of coverage. We have labeled each change of slope by a letter in rising order of appearance, as in Fig. 4. The solid lines are a guide to the eyes.

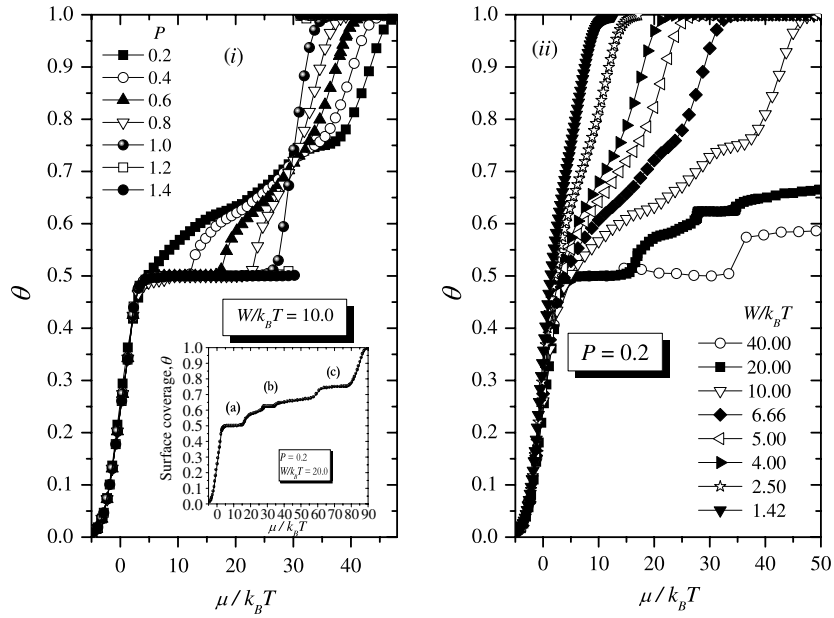

Fig. 7. (i) Adsorption isotherms for honeycomb lattice for a fixed temperature and different values of the non-additivity parameter, P, as indicated. The inset shows the isotherm for $P = 0.2$ at low temperature where the plateaus are clearly identified. We have labeled each plateau by a letter in rising order of appearance from (a) to (c). The same situation for $P = 0.2$ and several values of the reciprocal temperature expressed in units of W/k_BT as indicated.

formed. The maxima are labeled with the same methodology that the isotherms. For the regime (b) (where $P > 1.0$) a first order phase transition is observed as in the previously described case for triangular lattices. Thus, in Fig. 9 the adsorption isotherms for $P = 1.6$ and several temperatures are plotted. This transition is reported around $\theta = 0.72$. The inset shows $W_m(P)$. The above discussion for triangular lattice could be applied to the honeycomb lattice.

5. Conclusions

In the present work the traditional and widely used assumption of additivity of the interaction energy between adatoms for a lattice–gas system is replaced with a more realistic one for several experimental systems. We extended a previous study

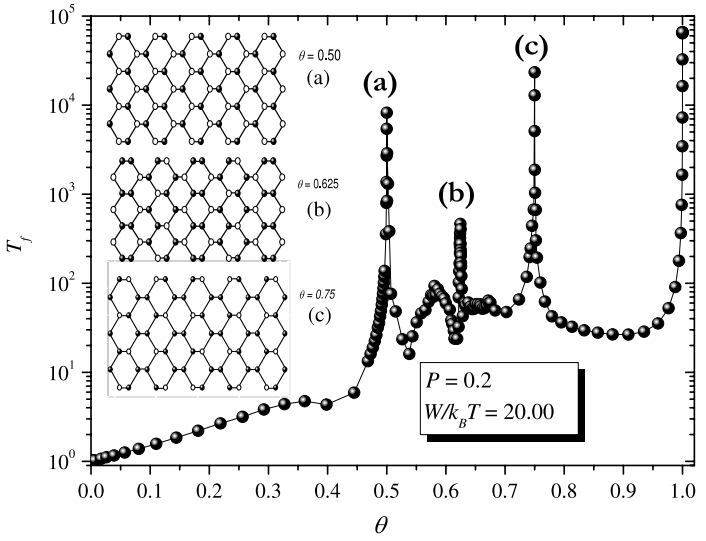

Fig. 8. Thermodynamics factor versus coverage for $P = 0.2$ and $W/k_BT = 20.0$. One can see how a narrow maximum appears at each coverage where the phases are established ($\theta = 1/2$, 0.625, and 0.75, respectively). In the upper left side of the figure typical snapshots of the low temperature phases (honeycomb lattice) are shown the ordered phases are plotted at: (a) $\theta = 1/2$, (b) $\theta = 0.625$ and (c) $\theta = 0.75$.

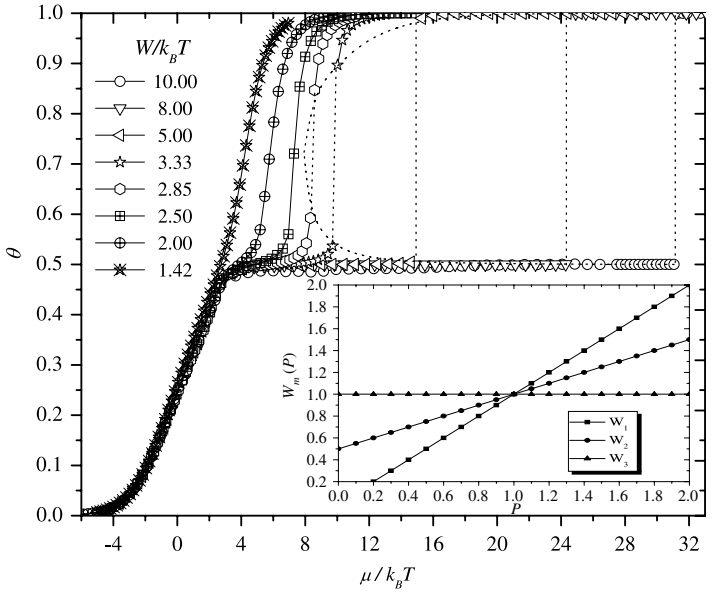

Fig. 9. Adsorption isotherms (honeycomb lattice) for $P = 1.6$ and different values of temperature expressed in units of W/k_BT. The dashed lines denote the coexistence area and they are shown only as a guide to the eyes.

of adsorption of monomers on square lattice, to triangular and honeycomb lattices. We supposed that the energy between nearest-neighbor depends on the state of occupation in the first coordination sphere of each adatom.

We have calculated the adsorption isotherms, thermodynamic factors, energy per site by means of Monte Carlo simulations in the grand canonical ensemble for triangular and honeycomb lattices. In the case where P is lower that one, it is possible to distinguish ordered phases at low temperature by depending on the surface coverage. The evidence of this affirmation is supported by (a) very wide plateaus in the adsorption isotherms, (b) peaks in the thermodynamics factor, (c) change of slope in the energy per site, (d) steps in the isosteric heat at the coverage where the phases are established. All this facts allow to conclude the existence of low temperature ordered phases for both lattices.

In the case of P larger than one it is found evidence of first order phase transition in the vicinity of $\theta = 0.72$ for the honeycomb lattice. In the triangular lattice there are evidence of two first order phase transitions at $\theta = 0.542$ from $\sqrt{3}\times\sqrt{3}$ to $(\sqrt{3}\times\sqrt{3})^*$ phase and $\theta = 0.80$–$(\sqrt{3}\times\sqrt{3})^*$ for filling the lattice.

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