Ordering and growth of rare gas films (Xe, Kr, Ar, and Ne) on the pseudo-ten-fold quasicrystalline approximant Al$_{13}$Co$_4$(100) surface

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Abstract
Adsorption of the rare gases Kr, Ar, and Ne on the complex alloy surface Al$_{13}$Co$_4$(100) was studied using grand canonical Monte Carlo (GCMC) computer simulations. This surface is an approximant to the ten-fold decagonal Al–Ni–Co quasicrystalline surface, on which rare gas adsorption was studied previously. Comparison of adsorption results on the periodic Al$_{13}$Co$_4$(100) surface with those of the quasiperiodic Al–Ni–Co surface indicates some similarities, such as layer-by-layer growth, and some dissimilarities, such as the formation of Archimedes tiling phases (Mikhael et al 2008 Nature 454 501, Shechtman et al 1984 Phys. Rev. Lett. 53 1951, Macia 2006 Rep. Prog. Phys. 69 397, Schmiedeberg et al 2010 Eur. Phys. J. E 32 25–34, Kromer et al 2012 Phys. Rev. Lett. 108 218301, Schmiedeberg and Stark 2008 Phys. Rev. Lett. 101 218302). The conditions under which Archimedes tiling phases (ATP) emerge on Al$_{13}$Co$_4$(100) are examined and their presence is related to the gas–gas and gas–surface interaction parameters.

Keywords: quasicrystalline approximant, ordering and growth, Archimedes tiling phases

(Some figures may appear in colour only in the online journal)

1. Introduction
Quasicrystals, unlike periodic crystals, may possess five-fold or ten-fold symmetry axes that produce five-fold or ten-fold diffraction patterns due to their positional and orientational symmetries [2]. Due to their extraordinary material properties [3], they have attracted much attention from researchers in the field, including studies directed at understanding the growth and ordering of atoms adsorbed on the quasicrystalline surfaces [6–13]. Experimental observations and Monte Carlo simulations of charged colloidal particles in a two-dimensional decagonal potential have produced much insight into the ordering, phase transitions, and other phenomena that occur for various interaction strengths, demonstrating a rich phase behavior that can provide insight into quasicrystal formation [4, 5]. One particularly interesting result is the existence of Archimedes tiling structures that occur over a very narrow range of density [4].

The adsorption of rare gases on quasicrystal surfaces has also proved to be a useful way of extracting valuable information on the growth of thin films, facilitated by the well-understood interactions involving rare gas atoms [14, 15]. Studies on the adsorption of rare gases on quasicrystalline surfaces indicated that, in the early stages of growth,
the rare gas follows the symmetry of the quasicrystalline substrate. At a later stage, however, the long-range order of the rare gas structure is adopted as long as the length scales defined by the gas atom size and the substrate structure meets certain conditions. Another class of materials, quasicrystalline approximants [6, 16], have the local structures of quasicrystals but also possess periodic long-range order. The periodicity of these materials greatly facilitates the determination of their surface structures, which can be determined precisely [17] without the need for extensive averaging or approximations [5, 18–21]. In an earlier electron diffraction study of the adsorption of Xe on the surface of the Al$_{13}$Co$_4$(100) quasicrystalline approximant [11], it was concluded that, similarly to Xe on the quasicrystal, the Xe initially takes the structure of the substrate, but achieves long-range order of nearly hexagonal symmetry at completion of the monolayer.

In this study, we have chosen the surface of the Al$_{13}$Co$_4$(100) quasicrystalline approximant, due to its ease of use compared to the quasicrystal substrate. One of the objectives of this work is to study the modes of growth on this surface as the size of the adsorbate decreases from Xe to Ne. Furthermore, we have studied the conditions under which Archimedes tiling structures can be formed in these rare gas films. Figure 1(a) depicts an idealized example of the type of Archimedes tiling observed in this study, in which the periodic length consists of two rows of triangles followed by two rows of squares, denoted as 2T2S.

The adsorption of Kr, Ar, and Ne on the Al$_{13}$Co$_4$(100) surface is investigated using grand canonical Monte Carlo (GCMC) simulations [9–11]. The Al$_{13}$Co$_4$ unit cell has lattice constants $a = 8.158$ Å, $b = 12.342$ Å, and $c = 14.452$ Å [22] and contains 102 atoms. Its structure consists of alternately flat (F) and puckered (P) layers of atoms parallel to its (100) surface, each separated by about 2 Å. The (100) surface structure was the subject of an extensive investigation using low-energy electron diffraction (LEED), scanning tunneling microscopy (STM) and density functional theory (DFT) [17], which concluded that it terminates in a P layer. The surface P layer is similar to its corresponding bulk layer, except for four missing Co atoms per surface unit cell. The structure of the surface P plane is presented in figure 1(b). The LEED pattern from this surface [17] displays a pseudo ten-fold symmetry, indicative of its close structural relationship to the ten-fold decagonal Al–Co–Ni quasicrystal surface.

2. Simulation procedure

A detailed description of GCMC applied to rare gas adsorption can be obtained from previous publications [9–11]. Briefly, the equilibrium number of adsorbed atoms $N$, at a volume $V$ and a temperature $T$, is determined using Metropolis Monte Carlo as a function of the chemical potential, $\mu$, of the adsorbed film. Provided that the film is in equilibrium with a sufficiently dilute gas reservoir, $\mu$ is related to the reservoir pressure $P$. **Figure 1.** (a) An idealized representation of type 2T2S Archimedean tiling. (b) Plot of the top layer atoms on the Al$_{13}$Co$_4$(100) surface. The drawing shows an area of four unit cells. In this surface layer, all the atoms are Al. The single (blue) atoms are denoted ‘glue’ atoms in the literature because they occur between bi-pentagons. For the remaining atoms, red (blue) denotes atoms that are below (above) the center of mass of the layer.
The interaction between the atoms was modeled using a Lennard-Jones 6–12 pair potential (LJ). The LJ parameters used here are given in Table 1. Figure 2 shows the calculated adsorption potentials for Kr, Ar and Ne, using the potential parameters given in Table 1. The potentials are superimposed over the structure model in Figure 1(b). The average potential energies are \(-125.3\) meV, \(-91.5\) meV, and \(-33.5\) meV for Kr, Ar, and Ne, respectively. These adsorption energies are smaller in magnitude than those reported for the same rare gases (Kr: \(-145.7\) meV, Ar: \(-113.3\) meV, and Ne: \(-47.4\) meV) on the Al–Co–Ni quasicrystal surface [8, 24]. The corrugation is, in general, also smaller than those on the Al–Co–Ni quasicrystal surface, except for Ne. One contributing factor for the smaller adsorption energy of rare gases on Al\(_{13}\)Co\(_4\)(100) as compared to the Al–Co–Ni quasicrystal surface is the absence of the Co atoms in the surface layer. It can be observed in Figure 2 that the strongest adsorptions sites for Kr, Ar and Ne occur at the centers of the lower (red) pentagons.

### 3. Simulation results

#### 3.1. Simulations of rare gases

The temperatures of the simulations were selected such that they are lower than the triple-point temperatures for the gas in each case. The same normalized temperatures \(T^* = T / \varepsilon_{gg}\) were used for each gas. For example, \(T^* = 0.35\) corresponds to temperatures of 80 K for Xe, 62 K for Kr, 43 K for Ar and 12 K for Ne.

**3.1.1. Kr adsorption.** The growth of Kr was simulated at temperatures of 62, 72, 82, and 92 K. The density plots for Kr on the Al\(_{13}\)Co\(_4\)(100) surface at a temperature of 62 K and the adsorption isotherm plot are shown in Figure 3. Figures 3(a)–(f)
correspond to the density plots at different stages of growth, which are marked on the adsorption isotherm. It is observed from the density profile and steps on the adsorption isotherm plots that the growth mode for Kr is layer-by-layer, however, the layering in the z direction is not as well defined as it is for Xe on the same surface [11]. The layers are also more corrugated as compared to the growth of Xe on the same surface. This layer-by-layer growth is a result of a weaker adsorbate–adsorbate surface interaction relative to the adsorption potential. The average density of the film is \( \rho = \frac{N_{av}}{A} \), where \( N_{av} \) is the average number of adatoms per layer and \( A = 713 \, \text{Å}^2 \) is the area of the unit cell. For Kr, \( \rho \) varies from 6.0 to 6.6 (atoms nm\(^{-2}\)) from the onset to the completion of the monolayer. In figure 3, it can be observed that at a fraction of monolayer growth (point A), only the centers of the red bi-pentagons are occupied. As the coverage increases to the onset of monolayer (point B), the minima at the centers of both the red and blue bi-pentagons are occupied. This indicates that Kr follows the quasicrystalline symmetry of the substrate at lower coverage. At the inception of the monolayer, the Kr structure can be described as an ATP [1–5]. This Archimedes tiling persists and appears to become more robust up to the completion of the monolayer. An ATP structure consisting of two rows of triangles and two rows of squares, 2T2S, is observed. From the Fourier transform graphs (figures 3(e) and (f)), it is observed that Kr acquires hexagonal symmetry at the beginning of the third layer, which persists to the point F on the isotherm.

3.1.2. Ar adsorption. Ar growth was simulated at temperatures of 43, 53, 63, and 73 K. All of these temperatures are below the Ar triple-point temperature of 83.81 K [23]. The density plots of Ar on the Al\(_{13}\)Co\(_4\)(100) surface at a temperature of 43 K, along with the adsorption isotherm plot, are given in figure 4. Figures 4(a)–(e) correspond to the density plots at different stages of growth, which are marked on the adsorption isotherm plot. From this density profile and the steps present on the adsorption isotherm graph, it is observed that the growth mode for Ar is layer-by-layer, with more defined layering than observed for Kr (see figure 3). From figures 4(a) and (b), it is observed that Ar follows the Al\(_{13}\)Co\(_4\) substrate at a fraction of monolayer coverage (point A) and the onset of the monolayer (point B). At the onset of the third layer, full hexagonal symmetry emerges and persists up to completion of the sixth layer.

3.1.3. Ne adsorption. The growth of Ne was simulated at a temperature of 12 K, which is below the triple-point temperature of Ne 24.55 K [23]. Density and adsorption isotherm plots of Ne on the Al\(_{13}\)Co\(_4\)(100) surface are given in figures 5(a)–(e). The adsorption isotherm has an inset of the density profile along the z-direction up to point E along the isotherm. From the lack of distinct steps in the adsorption isotherm, there is no strong indication that the growth mode is layer-by-layer, at least until significantly higher coverage, although some layering is evident in the density profile along...
Figure 4. Ar growth; density plots at various points on the adsorption isotherm. Unprimed letters correspond to density plots with bi-pentagons. Primed letters correspond to density plots with no bi-pentagons.

Figure 5. Ne growth; density plots as well as FFT at various points on the adsorption isotherm.

de in the z-direction. This is different from the growth mode of Xe, Kr, and Ar on the Al_{13}Co_{4} surface and for Ne on the quasicrystal substrate, where all the gases were observed to grow layer-by-layer at low coverage. In the sub-monolayer regime, Ne seems to follow the structure of the substrate, similar to the cases of Kr, Ar, and Xe. At point D on the
Figure 6. Xe_{d1} fictitious atom growth ($\sigma_{gg} = \sigma_{Kr-Kr}$); density plots at various points on the adsorption isotherm.

<table>
<thead>
<tr>
<th>Gas</th>
<th>($V_{min}(x, y)$)(meV)</th>
<th>$V_{min}(x, y)$ range (meV)</th>
<th>$\Delta \rho$ (atoms nm$^{-2}$)</th>
<th>$\sigma_{gg}$ (meV)</th>
<th>$\epsilon_{gg}$ (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Xe</td>
<td>$-152.9$</td>
<td>$-120$ to $-247$</td>
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<td>$6.0$</td>
<td>$6.6$</td>
</tr>
<tr>
<td></td>
<td>$(-195.5)$</td>
<td>$(-155$ to $-283)$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Kr</td>
<td>$-125.3$</td>
<td>$-85$ to $-193$</td>
<td></td>
<td>$6.0$</td>
<td>$6.6$</td>
</tr>
<tr>
<td></td>
<td>$(-145.7)$</td>
<td>$(-111$ to $-225)$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ar</td>
<td>$-91.5$</td>
<td>$-71$ to $-162$</td>
<td></td>
<td>$6.0$</td>
<td>$6.6$</td>
</tr>
<tr>
<td></td>
<td>$(-113.3)$</td>
<td>$(-85$ to $-181)$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ne</td>
<td>$-33.5$</td>
<td>$-26$ to $-74$</td>
<td></td>
<td>$6.0$</td>
<td>$6.6$</td>
</tr>
<tr>
<td></td>
<td>$(-47.4)$</td>
<td>$(-33$ to $-71)$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Xe_{d1}</td>
<td>$124.3$</td>
<td>$-97$ to $-204$</td>
<td></td>
<td>$6.1$–$6.5$</td>
<td>$3.60$</td>
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<tr>
<td>Ar_{i1e1}</td>
<td>$100$</td>
<td>$-78$ to $-177$</td>
<td></td>
<td>$6.9$–$9.2$</td>
<td>$3.60$</td>
</tr>
<tr>
<td>Ne_{i2e1}</td>
<td>$63.7$</td>
<td>$-49$ to $-112$</td>
<td></td>
<td>$7.0$–$8.3$</td>
<td>$3.60$</td>
</tr>
</tbody>
</table>

Table 2. Lateral average interaction potential of rare and fictitious gases on the Al$_{13}$Co$_4$ periodic substrate ($V_{min}(x, y)$), range of $V_{min}(x, y)$, range of densities over which ATP appear $\Delta \rho$, LJ parameters $\sigma_{gg}$ and $\epsilon_{gg}$ of the fictitious atoms. Where two numbers are given, the top number is from the present calculations on Al$_{13}$Co$_4$ and the lower numbers are results for adsorption on an Al–Co–Ni quasicrystal surface from [22].

isotherm, hexagonal symmetry emerges and persists up to point E.

3.1.4. Simulations of fictitious gases. Our simulations of rare gases on the Al$_{13}$Co$_4$(100) approximant indicate that only Kr exhibits AT, of type 2T2S, in the monolayer regime. Therefore, we believe that there is a very small range of densities of rare gas films, grown on the periodic Al$_{13}$Co$_4$ surface, that exhibit Archimedes tiling. The density of the film in the simulations can mainly be changed through the parameter $\sigma_{g-g}$ of the gas–gas LJ potential. The corrugation of the adsorption potential, which depends on the parameter $\epsilon_{g-g}$, can also affect the density of the film to a lesser extent. In order to verify our hypothesis concerning the formation of the AT, we defined some fictitious atoms that have the same $\sigma_{g-g}$ as Kr but the $\epsilon_{g-g}$ of Xe, Ar, and Ne, respectively. These fictitious atoms are referred to as Xe_{d1}, Ar_{i1}, and Ne_{i2}, respectively, where d1...
stands for a deflated Xe atom that has the \( \sigma_{g-g} \) of Kr. i1 and i2 stand for inflated Ar and Ne atoms that have the \( \sigma_{g} \) of Kr.

In order to investigate how the density of the adsorbed layer affects its structure we first constructed potentials between the fictitious atoms and the substrate. The LJ potential parameters between the fictitious atoms along with the well depth of the laterally averaged rare gas substrate potentials and their corrugations are tabulated in table 2. These potential parameters along with the LJ potentials for the adsorbate–adsorbate and substrate–substrate atoms were used as input to the GCMC simulations. We conducted three simulations for the three fictitious atoms Xe\(_{d1}\), Ar\(_{i1}\), and Ne\(_{i2}\) at temperatures 80, 43 and 12 K, respectively. Out of the three fictitious atoms only simulation of Xe\(_{d1}\) produced ATs of type 2T2S in the monolayer regime. The simulation of Ar\(_{i1}\) produced ATs of type 3T1S. This appears to be a mechanism that allows a film to accommodate higher density while maintaining Archimedes symmetry. The results for the density and adsorption isotherm plots of Xe\(_{d1}\) are reported in figure 6. The density plots for Xe\(_{d1}\) correspond to points A, B, and C on the isotherm and the density profile corresponds to point D. From the density plots in figure 6, it is clear that growth of the fictitious atom Xe\(_{d1}\) on the Al\(_{13}\)Co\(_{4}\)(100) approximant results in Archimedes tiling with 2T2S patterns. The range of \( \rho \) for the adsorbed Xe\(_{d1}\) film, from the onset to the completion of the monolayer, for forming ATP is reported in table 2.

To check the effects of \( \epsilon_{g-g} \) on the emergence of ATP, we defined two more fictitious atoms Ar\(_{i1e1}\) and Ne\(_{i2e1}\). Ar\(_{i1e1}\) represents a fictitious atom with the \( \sigma_{g-g} \) of Kr and an \( \epsilon_{g-g} \) that satisfies \( \epsilon_{Ar-Ar} < \epsilon_{g-g} < \epsilon_{Kr-Kr} \). Ne\(_{i2e1}\) represents a fictitious atom with the \( \sigma_{g-g} \) of Kr but an \( \epsilon_{g-g} \) that satisfies \( \epsilon_{Ne-Ne} < \epsilon_{g-g} < \epsilon_{Ar-Ar} \). The GCMC simulation results of Ar\(_{i1e1}\) and Ne\(_{i2e1}\), at temperatures 43 K and 12 K, are presented in figures 7 and 8, respectively. It is observed from figures 7 and 8 that fictitious atoms Ar\(_{i1e1}\) and Ne\(_{i2e1}\), with the specific values of the parameters \( \sigma_{g-g} \) and \( \epsilon_{g-g} \), reported in table 2, exhibit ATP of type 2T2S. The range of densities of the Ar\(_{i1e1}\) and Ne\(_{i2e1}\) films (in the monolayer regime) for the emergence of ATP are reported in table 2. Our results corroborate two conditions, set forward in [4], for the emergence of Archimedean tilings; a narrow density range of adsorbate and an intermediate potential strength of the adsorbate–substrate potential.

The density of the adsorbed monolayer versus the strength of the adsorbate–substrate potential for which ATP of type 2T2S occur are graphed in figure 9 for various elements and temperatures for which simulations were carried out. The horizontal and vertical axes in figure 9 represent the unitless quantity \( V_{o}/(k_{B}T) \) (where \( V_{o} = \langle V_{min}(x,y) \rangle \)) and the number density \( \rho \) of the adsorbed atoms in units of \((\text{atoms nm}^{-2})\), respectively. The length of each bar represents the range of the density of the adsorbed layer in the monolayer regime, for the observation of ATs of type 2T2S. The phase diagram in figure 9
indicates that ATs of the type 2T2S are indeed observed for a narrow density of the overlayer and intermediate potential strengths. This trend for the occurrence of Archimedes tiling in figure 9 is similar to that of [4].

In layer-by-layer growth, the isosteric heat of adsorption per atom at fixed coverage \( n \) is defined by [10]:

\[
q_{st} = -k_B \left( \frac{\partial}{\partial T} \ln P \right) \left( \frac{1}{n} \right)
\]

where \( k_B \) is the Boltzman constant. In figure 10, plots of \( \ln(P) \) versus \( 1/T \), from the simulations along with best fitted lines, are presented for Kr and Ar. There are two coverages for each system; onset of the first monolayer \( (n = 1) \) and onset of the second monolayer \( (n = 2) \). The isosteric heats thus derived are reported in table 3 for Kr and Ar on the Al\(_{13}\)Co\(_4\) surface at different coverage. To the best of our knowledge, no experimental data is available for the isosteric heats of adsorption of Kr and Ar on this surface. However, the P termination of the Al\(_{13}\)Co\(_4\) approximant that was employed in this study includes only Al atoms and is, therefore, similar to an Al surface. Due to the similarities of these two surfaces, it is therefore reasonable to compare our results with those for the adsorption of Kr and Ar on an Al(111) surface. Isosteric heat values of 185 meV and 143 meV have been reported for the onset of the first monolayer on the Al(111) surface for Kr and Ar respectively [25]. These values fall within the range of our calculated isosteric heat values of 191 meV, 112 meV and 147 meV, 83 meV, respectively, for the first and second layers of Kr and Ar.

### Table 3. Isosteric heat of adsorption \( q_{st} \) for the various systems studied here. \( q_{st} \) is in meV. \( n \) is in fractions of a monolayer.

<table>
<thead>
<tr>
<th>System</th>
<th>( q_{st} )</th>
<th>( n )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ar/Al(_{13})Co(_4)(100)</td>
<td>147</td>
<td>1</td>
</tr>
<tr>
<td>Ar/Al(_{13})Co(_4)(100)</td>
<td>83</td>
<td>2</td>
</tr>
<tr>
<td>Kr/Al(_{13})Co(_4)(100)</td>
<td>191</td>
<td>1</td>
</tr>
<tr>
<td>Kr/Al(_{13})Co(_4)(100)</td>
<td>112</td>
<td>2</td>
</tr>
</tbody>
</table>

### 4. Summary and discussion

Our simulation results indicate that Kr and Ar grow layer-by-layer on the complex metallic alloy surface Al\(_{13}\)Co\(_4\)(100), at least for the first few layers. On the other hand, the structure of Ne seems to be sufficiently disrupted by the substrate potential such that it does not follow an orderly growth. Interestingly, the growths of Kr, Ar and Ne on Al–Ni–Co quasicrystal surface are all layer-by-layer. At lower coverages, Kr, Ar and Ne all follow the symmetry of the periodic surface, while at higher coverages they will eventually exhibit the hexagonal symmetry of the particular rare gas. This is similar to the growth on the quasicrystal surface.
Figure 9. Phase diagram for the occurrence of type 2T2S Archimedes tiling.

Figure 10. Plots of ln(P) versus 1/T, from the simulations along with best fitted lines used in the calculation of the isosteric heat of adsorption, are presented for Ar and Kr.

The main result of this work is that Kr in the monolayer regime, from onset to completion, exhibits ATP of type 2T2S. This growth mode is absent for other rare gases on the periodic surface. In comparison, the ATP phase was not observed for any of these rare gases (Xe, Kr, Ar, and Ne) on the Al–Ni–Co quasicrystal surface. In an earlier simulation study of rare gases on the Al–Ni–Co quasicrystal surface, the emergence of long-range order of the film depended on the value of the LJ parameter $\sigma_{gg}$ of the rare gas. If $\sigma_{gg}$ of the rare gas is greater than the $\sigma_{gg}$ of Xe, then long-range order will emerge. Our simulation results indicate that for the emergence of the ATP phase the $\sigma_{gg}$ of the rare gas atom needs to be close to the $\sigma_{gg}$ of Kr, whereas the $\varepsilon_{gg}$ can be somewhat higher or lower than the $\varepsilon_{gg}$ of Kr.

To summarize, we have studied the adsorption of rare gases on the Al$_{13}$Co$_4$ (100) surface using GCMC simulations, and compared the results with earlier studies on Xe on the Al$_{13}$Co$_4$ (100) surface as well as these rare gases on the Al–Co–Ni quasicrystalline surface. The growth mode on these two surfaces is, generally, layer-by-layer and the overlayer takes the symmetry of the substrate at the lower coverages, but eventually takes hexagonal symmetry at higher coverages. The growth of a Ne film on the periodic surface differs by not exhibiting a sharp layer-by-layer growth. The growth of Kr on the Al$_{13}$Co$_4$ (100) surface exhibits an ATP phase at the onset of the monolayer that persists up to the completion of the monolayer. This behavior was not observed on the Al$_{13}$Co$_4$ (100) surface for other rare gases. The present work indicates that the determining factors in the emergence of ATP are the density of the adsorbed layer as well as the strength of the adsorbate–substrate interactions. Unlike the growth of rare gases on the Al–Co–Ni quasicrystalline substrate, which produces quasicrystalline symmetry in the monolayer regime for a range of rare gases, the growth of rare gases on the Al$_{13}$Co$_4$ (100) surface results in ATP only in a narrow range of densities and intermediate adsorbate–substrate potential strengths. Based on our simulations, Kr has the optimal density for producing ATP. Growth of Ar, Ne and Xe on
the Al$_{13}$Co$_4$(100) surface does not seem to have the specific density for the emergence of ATP. However, by simulation of some fictitious atoms with densities close to that of Kr and with intermediate strengths, emergence of ATP was observed.

Finally, we have calculated the isosteric heat of adsorption for Kr and Ar on the Al$_{13}$Co$_4$(100) surface. Our calculated isosteric heats of adsorption values for the first two layers (191 meV and 111 meV for Kr and 147 and 83 meV for Ar) are consistent with the monolayer heats of adsorption of Kr and Ar on the Al(111) surface (185 and 143 meV).

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