Adsorption of Multiple Spherical Particles onto Sinusoidally Corrugated Substrates

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1 Supporting Information

ABSTRACT: We utilize a Monte Carlo simulation scheme based on the bond fluctuation model to simulate settlement of adhesive particles onto sinusoidally corrugated substrates. The particles are composed of a hard inner core with either an effective potential shell or a “soft” adhesive shell made of flexible arms attached to the particle surface. These chains adhere via either the effective potential shell or the sticky chain ends to the surface via pairwise nonspecific interactions. This simulation model allows for multiple particles to settle onto each tested substrate to elucidate the behavior of the collective adhesive layer featuring multiparticle assembly. Particles move within a 3D lattice space and settle on the substrate due to attractive particle/substrate interactions. Once a single particle adheres to the substrate, a new particle is introduced into the lattice to begin a new settlement. Through this multiparticle settlement mode, we explore the interplay among the characteristics of the particles (i.e., size, interaction shell) and the substrates (i.e., wavelength and periodicity) as well as interparticle interactions. We report that the adhesion of particles with an effective interaction shell to the substrates is reduced dramatically when the particle size is smaller than the feature width of the periodic substrate. The settlement of particles with flexible hair on the sinusoidally corrugated substrates is more complex. Specifically, the presence of flexible polymeric hairs makes the particle settlement more likely to occur on nearly all substrates studied irrespective of the characteristics of the substrate.

1. INTRODUCTION

The settlement and organization of particles with adhesive surface groups onto material substrates is important to many fields of science and technology ranging from biofouling to particle sorting.1−16 In this work, we focus on comprehending the adsorption of multiple spherical particles onto topographically corrugated substrates featuring sinusoidal patterns. The particles studied here interact with the substrate via either an effective field or surface-grafted polymer arms featuring “sticky” end-groups. For the case of effective interaction field, we also address the interplay between the particle/substrate versus particle/particle interactions. Such systems are particularly relevant to the adsorption of bacteria and other small biological organisms (i.e., cyprids or zoospores) that interact not only with the substrate but also with one another when settled on surfaces (i.e., they may form biofilm layers). This work aims to understand the role periodic substrate topography plays in governing the adhesion of fouling particles. While there are areas that seek to promote adhesion of particle-like adsorbates (i.e., cell adsorption or particle sorters), in many fields, specifically in biofouling, most efforts have aimed at reducing the adsorption of foulers via chemical methods.17−21 For example, ethylene glycol17,18,22 or some charge-bearing surfaces23−25 are capable of minimizing (at least temporarily) bioadsorption on material substrates. Utilizing substrates with engineered surface topographies provides an alternative means toward enhancing the resistance of materials surfaces for fouling by controlling the number of interaction points between the “foulant” and the adsorbing surface. Nature provides ample inspiration for controlling the extent and strength of adsorption on nano- and microstructured substrates. One of the most notoriously known examples is the Lotus leaf that creates a superhydrophobic surface by minimizing the number of contacts between the adsorbing hydrophilic liquid, such as water, and the substrate through the combination of waxy hydrophobic residues on nanostructured substrate features and their spatial arrangement on the substrate.26−28 The symbiosis between the chemical and topographical properties of the Lotus leaf endows it low adhesiveness and self-cleaning characteristics.26 Several studies have explored experimentally the application of textured surfaces in preventing biological adhesion. Examples include the Sharklet patterns,29 hierarchical wrinkles with multiple dimensions,1,30 corrugated periodic structured substrates,18,25,29,31−35 or substrates with random topographical features. Despite these efforts, very little is understood about the types of topographical morphologies and their dimensions that are best suited to reduce biofouling. Some studies have alluded to contact point theory29,31,32,36−38 and investigated sinusoidal
topographies with promising results; yet those studies did not develop a substantial theoretical basis for predicting fouling behavior.

Figure 1. Simulation setups and particle parameters including particle size (\(D\)), grafting density of hairs (\(\sigma\)), length of hairs (\(N\)), and the hair/substrate interaction parameter (\(\varepsilon\)).

Figure 2. Positions of hard sphere particles (\(D = 20\)) on sinusoidally corrugated substrates with variable amplitude (\(A\)) and variable feature width (\(\lambda\)). Amplitude decreases moving down, while feature width decreases moving right. Core of particles shown in blue-green, higher substrate features are lighter, and lower surface features are darker.

Given the large set of system parameters governing the adsorption of particles on topographically corrugated surfaces, comprehending the role of each individual parameter as well as...
their mutual interplay is not straightforward. One way to gain more insight into this phenomenon is to develop a predictive computational model that would facilitate systematic variation of the individual parameters and narrow the vast parameter set that would eventually be studied in experiment. We have developed a Monte Carlo computer simulation scheme to model the adsorption of particles interacting with surfaces featuring sinusoidally corrugated topographies. In our model, the fouling particles are simulated as hard core species that exhibit either an implicit interaction field or an explicit set of “sticky” surface-grafted polymer arms that interact with the underlying substrate. We modify the frequency and amplitude of the substrates and study their effects on the adsorption of particles with variable particle diameter. In the implicit particle model, we also vary the particle adhesion to the substrate as well as interparticle interactions. In the explicit adsorption particle model, we explore the effects of the grafting density of adhesive hairs, length of hairs, number of adhesive hairs per units area, and energy per polymer coarse-grained element-to-surface contact.

2. COMPUTER MODEL AND DATA ANALYSIS

Hard Sphere Particles (Implicit Interaction Shell). First, we employ a Monte Carlo simulation scheme to model the behavior of adhesive hard sphere particles on substrates featuring sinusoidal profiles defined by their amplitude and frequency/wavelength. In this work, we refer to the frequency and wavelength as surface feature width and amplitude as feature height, respectively. The spherical particles interact with the corrugated substrates via nonspecific interactions in an effective interaction shell around the particle. Adhesion energies are counted by summing the number of surface lattice points within the effective interaction shell. These particles are allowed to perform one move per MC step (MCS) in one principle direction (i.e., ±x; ±y; and ±z) within a lattice. After each MCS, the adhesion energy is calculated and recorded as well as the spatial location of said particle. System testing was performed at a high number of MC steps to ensure particles were able to reach multiple maxima in their allotted settlement time. After this time, the location, where the particle achieves its highest adhesion energy, is considered as its settled location on the substrate. Particles are inserted onto the lattice sequentially, meaning only one particle moves at any time and all settled particles remain stationary. The simulation is complete once all available substrate area is taken by the settled particles and no new particles can settle on the surface.

“Soft” Sphere Particles (Explicit Polymer Layer). In addition, we employ a MC simulation scheme to model the behavior of adhesive hard sphere particles covered with explicit polymeric “hairs” interacting with the substrates through their sticky ends. The particle movements are regulated by the bond fluctuation model (BFM). The system features a cubic lattice comprising 160 × 160 × 200 lattice cells versus the 500 × 500 × 200 lattice cells used in our other work. Larger lattices with more particles were tested but did not show a significant deviation in results; thus, for the sake of computational time, smaller lattices were used. BFM dictates a set of 108 possible bond vectors allowed in a cubic lattice as shown by the set of moves: P(2,0,0) U P(2,1,0) U P(2,1,1) U P(2,2,1) U P(3,0,0) U P(3,1,0) and their permutations and sign inversions of such. All moves in the BFM are selected randomly and attempted with favorable moves tending toward an increase in adhesion energy. To strike a balance between the entire particle moving and each element of the surface-grafted polymer elements moving on the lattice, we operate each on different time scales. In this simulation, we use MCS as “time”. The set of possible moves in this system consists of coarse-grained polymer chain moves and movement of the entire particle.
Polymer chains move on a faster time scale than that of the moves of the overall particle; thus the move probabilities are balanced as such. There is no preferential direction imposed on the movement of the particles; that is, no gravitational or other external forces affect the motion of particles as they move within the lattice. Changes to adhesion energy of the system are handled by the Metropolis MC decision algorithm where any move that increases the interaction energy is accepted and any move that causes a decrease in interaction energy is accepted with the probability proportional to $e^\frac{\Delta E}{kT}$, where $\Delta E$ is $E_{\text{system}} - E_{\text{system,i-1}}$ (note the difference in sign convention as this deals with energy of adhesion, which we treat as a positive quantity, and thus the algorithm seeks to maximize energy of the system). This simulation scheme maintains randomness in the system and allows each particle to escape local energy minima. Each particle trial is given an arbitrary amount of time to first equilibrate the flexible arms anchored to the particle surface before the particle itself is allowed to move as a whole; we use 1000 MCS per polymer coarse-grained element. After being inserted into the lattice, each particle moves freely in any direction, and the simulation ends after a predetermined set of MCSs. The number of MCS is adjusted on the basis of long time energy equilibrations such that each particle reaches several energy maxima; this results in $\sim$10 000 MCS per chain element in these simulations. The particle is considered settled at whichever location on the substrate when it achieves its highest adhesion energy throughout its entire simulation time. The particles settled on the substrate remain stationary. The only moving particle is the newest particle searching for a location on the substrate to settle on. We do not increase the allotted MCS for new particles because the total number of MCS was equilibrated such that a single particle has plenty of time to explore a large area and reach several maxima, thus given reasonable time that all particles must adhere to. The simulation ends once 10 consecutive particle trials have failed to attach to the surface. We note that in our model, a particle is considered to be adhered to the substrate if it is in a direct contact with the substrate. Thus, in determining the strength of particle adhesion, we do not account for particles in multilayer assemblies that are not attached directly to the substrate. In simulating multiparticle settlement through adsorption of individual particles, we maximize the adhesion energy between each particle and the substrate and thus the overall adhesion. As will be evident from the results, particles tend to close-pack on the substrate, which validates our approach. It would be interesting to compare the results of this model to a scheme, which considers concurrent motion of all particles. This, however, is outside the scope of the current work.

Figure 1 provides the layout of the simulation setup and defines the parameters of the corrugated substrate and the particles employed in the simulation. Specifically, the substrates comprise sinusoidal topographies with adjustable amplitude and wavelength, referred to later as feature height and feature width, respectively. Data discussed in this Article include a set of three feature heights and six feature widths, which when combined create 18 unique surfaces for each set of particle conditions tested. The explicit particles are defined by their core diameter ($D$), number of repeat segments in the anchor arms ($N$), grafting density of arms, that is, the number of arms per unit area, on the particle surface ($\sigma$), and the interaction potential acting between the last two adhesive segments of the flexible “hair” and the surface ($\epsilon$). In the implicit particle simulation, we vary the particle/particle interaction energies. During the MC simulation, we track positional data of all anchored arms and the center of mass of the particle as well as the current adhesion energy of the system. Each data point presented is the result of three identical simulation sets.

3. RESULTS AND DISCUSSION

Hard Sphere Particles. Figure 2 depicts examples of hard core particles ($D = 20$) settling on substrates comprising four different feature heights ($A$) and six different feature widths ($\lambda$). The particles experience an effective interaction shell potential with the substrate but no particle/particle interactions. Particles settling on substrates with large feature widths cover the entire available substrate relatively uniformly. Decreasing $\lambda$ lowers the available surface area on the substrate onto which the particle can settle. In particular, for $\lambda = 40$ and 20, the particles are blocked completely from entering the valleys of the substrates; this effect gets even more exaggerated with increasing $A$. At $\lambda = 20$, the feature width matches the particle size; the particles assume well-defined positions on the substrate that are dictated by the substrate features (i.e., $A$ and $\lambda$). This trend continues also for substrates with $\lambda < D$. For $\lambda \ll D$, a case not studied here in detail because of finite lattice size effects, one would expect that the particles would lose completely the memory of the substrate features and would settle relatively randomly on...
the substrate. In Figure 3 we plot the adhesion energy of particles with $D = 20$ with the effective interaction shell settling on surfaces featuring four different values of $A$ and six different values of $\lambda$. The adhesion energy per particle relative to that for a flat substrate is plotted for each data set as a function of the average particle counter, that is, the number of particles settling on each substrate. Regardless of the substrate feature width and feature height, we detect that particles arriving to the substrate in early stages of the adsorption process experience higher adsorption energy relative to particles that arrive to the substrate at later times. For $\lambda \gg D$, the adhesion energy decreases continuously until a certain particle number threshold indicating the point at which the particles saturate the substrate and can no longer find a site to which they can adsorb. For $\lambda \approx D$ and $\lambda \ll D$, the adhesion energy is relatively constant in the initial stages and reaches the same threshold mentioned above. In addition, we notice that while for $\lambda \gg D$ the adsorption is governed primarily by $\lambda$ (in the latter stages of adsorption), the adsorption of particles whose diameter is comparable to $\lambda$ is governed by $A$ (in the initial stages of adsorption). Adsorption in the $\lambda \ll D$ regime is independent of $A$ and $\lambda$. The data in Figure 3 confirm the trends we discussed earlier with regard to Figure 2.

The total adsorption energy of particles on substrates can be obtained by integrating the respective curves in Figure 3. In Figure 4a we plot the total adhesion energy on corrugated substrate relative to adhesion on a flat substrate as a function of the feature width scaled in terms of the particle diameter for substrates with a variable $A$ and $\lambda$. For $\lambda \gg D$, the adhesion is comparable to that on flat substrates, as expected. Decreasing $\lambda$ leads to higher adsorption energies of the particles because of increased surface area on the substrate, which results ultimately in higher particle accumulation on the substrate and higher total adhesion energy. When $\lambda$ approaches the particle size, the particles are excluded from penetrating the substrate topography, which results in smaller particle settlement and ultimately lower overall adhesion energy. For $\lambda < D$, the particles are not able to penetrate efficiently the valleys of the substrate features; yet, the memory of the substrate is not lost completely because even a very small particle penetration into the substrate is capable of ordering the particles on the substrate by following the underlying topographical pattern. We mentioned earlier that for $\lambda \ll D$ one would expect the particles to adsorb in a manner that is similar to that on flat substrates. Finite lattice size effects, however, preclude us from probing this regime effectively. In fact, lattice effects may play a role, in general, in these simulations.

**Figure 5.** Positions of hard sphere particles ($D = 20$) on sinusoidally corrugated surfaces with constant amplitude ($A = 80$) and variable feature width ($\lambda$). Interparticle interactions increase from top to bottom. Core of particles are shown in blue, higher surface features are lighter, and lower surface features are darker.
The particle/particle interactions (E\textsubscript{PP}) excluding any e\(\lambda\) however, for the particle is relatively high for substrates featuring small \(\lambda\) irrespective of \(\lambda\). A variable adhesion per particle decreases with decreasing the total number of particles settled on the substrate. The data in Figure 4b depict such a situation. We see that, generally, the adhesion per particle decreases with decreasing the \(\lambda/D\) ratio irrespective of \(A\). For \(\lambda/D \approx 1\), the adhesion energy per particle is relatively high for substrates featuring small \(\lambda\); however, for \(\lambda/D \ll 1\), the adhesion of particles on the surfaces decreases dramatically for all substrate regardless of the feature height. This result suggests that adhesion of particle in systems featuring \(\lambda/D \ll 1\) is lower than that on flat substrates and reveals that utilizing topographies featuring sinusoidally corrugated substrate topographies with feature widths smaller than the particle diameter is efficient in decreasing the settlement of particles that interact with the substrate with an effective shell interactions.

During the MC simulations, we monitor the spatial distribution of the adsorbed particles on the various substrates for all combinations of feature widths, feature heights, and interparticle interactions. Figure 5 denotes a map of the positions of particles settling on substrates with the same \(\lambda\) and variable \(\lambda\) for three strengths of particle/particle interaction. The particle/particle interactions (E\textsubscript{PP}) are expressed as a fraction of the particle adhesion strength to the substrate (E\textsubscript{PS}). Using such location maps, we gain information about how the spatial organization of particles on substrates is influenced by the underlying substrate topography and particle/particle interactions. The data in Figure 5 demonstrate visually that the particles settle predominantly inside the valleys of the substrate topographical features that offer the largest available substrate area through which the particles can interact with the substrate. This behavior is pronounced on substrates featuring large \(\lambda\). Decreasing \(\lambda\) of the substrate decreases the area of the substrate available for adhesion of the settling particles and, in turn, leads to lower particle settlement. When \(\lambda\) of the substrate protrusions becomes comparable to or smaller than \(D\), the number of particles decreases dramatically; this process is associated with dramatic reduction of the adhesion energy (cf., Figure 4 for \(E_{PP} = 0\)). For \(E_{PP} = 0\), the particles still reside above the valleys of the substrate but are more separated. Increasing the strength of the particle/particle interactions does not alter the general trend for particle location observed for \(E_{PP} = 0\); that is, the particles settle predominantly inside the valleys of the substrate. However, unlike the situation of for “athermal” particle/particle interactions (i.e., \(E_{PP} = 0\)), increasing \(E_{PP}\) results in additional ordering of the particles in the plane of the substrate. Specifically, increasing \(E_{PP}\) causes the particles to close-pack locally. Depending on \(\lambda\), this close packing takes place either inside the surface valleys (\(\lambda \gg D\)) or across the entire substrate (\(\lambda \ll D\)). The latter organization, which often features hexagonal close-packing, demonstrates clearly the intimate
interplay between the particle organization driven solely by the substrate topography and that originating from the particle/particle interactions. Specifically, increasing the strength of the particle/particle interaction causes an increase in the tightness of packing, which enables more particles to settle on the substrate. Interestingly, the substrate least affected by this has feature spacing equal to the diameter of the particle.

More insight into particle settlement on sinusoidally corrugated substrates can be obtained by examining the sequence of arrival of individual particles to the substrate and the role of the particle/particle and particle/substrate adhesion on particle settlement on the surfaces. In Figure 6, we plot the order in which the particles adsorb on the substrates. The data are depicted by color; that is, the first group of particles arriving to the substrate is depicted in red, while the last group of particles settling is marked in blue. The order of particle settlement depends on both the nature of the substrate and the particle/particle interactions. We start by discussing the case of particle arrival time more. In situations involving strong particle/particle interactions (right column in Figure 6), the particle settlement, even on flat substrates, depends on the strength of particle/particle interactions. Particles settle in clusters of relatively close-packed (large $\lambda$) to very close-packed (small $\lambda$) arrays, indicating that increasing the strength of particle/particle interactions forces the settled particles to assume positions close to the already adsorbed neighbors. Figures 7 and 8 provide further evidence of the importance of particle/particle and particle/substrate interactions, respectively, on particle settlement. The plots in Figure 7 demonstrate that the number of interparticle contacts increases with increasing particle/particle interaction energy. For the strongest interparticle interactions and substrates that are either flat ($\lambda = \infty$) or tend to make the particles reside in a single plane ($\lambda = 5$), the particles tend to adopt close hexagonal packing (i.e., 6 nearest neighbor contacts). Figure 8 depicts the effect of particle/substrate interaction on particle adhesion on various substrates. There are no major trends among the various $E_{pp}$ values and various substrate features.

**“Soft” Sphere Particles.** In addition to MC simulations involving particles that exhibit implicit interactions with the substrate, we also simulated the adsorption of particles covered with explicit polymeric hairs. In Figure 9, we plot the positions of particles with $D = 20$ coated with polymer arms with the length ($N$) of 3 segments and grafting density ($\sigma$, i.e., the number of polymers per unit area) equal to 0.1 on substrates with three different feature heights and six different feature widths. Just like in the case of adsorption of particles with implicit interaction shell, the particles with explicit interaction sites tend to adsorb preferentially inside the valleys of the substrate protrusions on substrates with relatively large feature width. Decreasing the width of the substrate reduces the available space on the substrate to which the particles can attach, and, in turn, reduces the number of settled particles. The latter behavior is more pronounced for substrates whose $\lambda$ becomes comparable to or smaller than the particle size ($D$). Here, the particles are excluded from penetrating inside the substrate valleys and settle primarily on all areas of the substrate surface.

In Figure 10, we plot the adhesion energy of particles with $D = 20$ with the explicit polymer hairs ($N = 3$, $\sigma = 0.04$) adsorbing onto substrates featuring three different values of $A$ and six different values of $\lambda$. The adhesion energy per particle relative to that for a flat substrate is plotted for each data set as a function of the average particle counter, that is, the number of particles settling on each substrate. The general trends are similar to those reported earlier for the settlement of particles with an effective interaction potential with a few exceptions. Particle adhesion increases with decreasing $\lambda$, due to increased substrate area available for particle adsorption, peaks at $\lambda = 40$, and then decreases with decreasing $\lambda$. The adhesion of particles on substrates with $\lambda < D$ is similar to that observed in particle settlement on flat substrates. For each feature width, the particle arriving at early stages of the adsorption process settle relatively strongly, while particles adsorbing in the late stages experience weaker adsorption to the substrate due to limited space on the substrate to which they can settle. Unlike in the case of an effective interaction potential, where we noticed amplitude-dependent adhesion, in all cases studied here the amplitude does not seem to make a difference. In addition, the abrupt decrease in adhesion mentioned earlier for the case of particles with effective interaction potential in the late stages of adsorption is not present in here. Clearly, the presence of flexible hairs on the surface of the particles governs particle adsorption; it acts as a mediator during the adsorption process.
A more quantitative picture of particle adhesion energy is obtained by determining the total adhesion energy of particles by integrating the areas under the respective curves in Figure 10. Figure 11 depicts the total adhesion energy (a) and the adhesion energy per particle (b) as a function of $\lambda/D$. The data are colorized on the basis of the number of particles adsorbed. The plots feature results of averaging a set of three identical simulations for each condition ($A$ and $\lambda$ of substrate). The trends in the total adhesion energy of particles are similar to those observed for the adsorption of particles with an effective potential shell.
Figure 11. (a) Total adhesion energy and (b) adhesion energy per particle for particles covered with polymeric hair ($N = 3, \sigma = 0.04$) adsorbing onto sinusoidally corrugated substrates as a function of feature width ($\lambda$) normalized by the particle diameter ($D$) for substrates featuring different amplitudes ($A$) and two different particle sizes. The color scale represents the number of particles adhering to the given substrate (blue = highest, red = lowest). The particle diameter is $D = 20$.

For $\lambda/D \gg 1$, the total adhesion energy is similar to that detected for particles adsorbing on flat surfaces. With decreasing $\lambda/D$, the total adsorption energy and the total number of adsorbed particles increase relative to that on flat substrates as $\lambda/D$ approaches unity; this increase is more pronounced for particles adsorbing on substrates with higher $A$. A maximum in the total adsorption energy is reached at $\lambda/D \approx 2$; further decrease in $\lambda/D$ results in lower total adsorption energy of particles (relative to flat substrates). Recall that in the case of effective interaction shell potential, the maximum adhesion is reached when $\lambda \approx 2D$; similarly for the present case involving the adsorption of particles with explicit polymeric hairs, the highest adsorption appears at $\lambda \approx 2D$. This is because in the latter case the particle diameter is effectively increased by the presence of the flexible hairs. The results in both cases are thus consistent and reveal that the maximum adhesion occurs when the particle size matches approximately the feature width of the substrate protrusions. By normalizing the total adsorption energy of particles to the adsorption energy per particle, the data in Figure 11a decreasing coincide with the adsorption of “hairy” particles on flat substrates (Figure 11b). We attribute this behavior, in large part, to the “softness” of the adsorbing particles that can readily adapt to variations of the local topography of the substrate. The trends observed here are consistent with those reported for the adsorption of a single “hairy” particle. Specifically, in addition to the size of the particle itself, the presence of the flexible polymeric hair anchored to the substrate of the particle determines greatly the extent of particle adsorption on topographically corrugated substrates. Particles with long and dense flexible arms adsorb heavily on topographically corrugated substrates; the extent of adsorption increases with increases in grafting density of the flexible adhesive arms and their length.

4. CONCLUSION

We have explored the settlement of both hard spherical particles with an effective interaction potential and those with flexible surface-anchored arms on topographically corrugated substrates featuring sinusoidal shapes of varying feature height and feature widths. In addition to exploring the interplay between the particle size and the aforementioned attributes of the substrates, we also investigated the roles particle/particle interactions on surface organization of the settled particles. The major conclusion from this study is that the number of settled particles on the substrate depends critically on the interplay between the size and nature of the adsorbing particle and the characteristics of the underlying substrate. While substrates with relatively large substrate feature promote particle adhesion, reducing the feature width of the substrate to (or slightly below) the particle size decreases dramatically the number of particles settled and their adhesion to the substrate. We also addressed the role of interparticle interactions on settlement on substrates. Specifically, we established that in cases involving strong particle/particle attraction, the particles aggregate on substrates in close-packed arrays. We have also documented that the structure of the interacting groups governing the adsorption of the particles to the substrate plays a major role in determining the adhesion of particles to underlying substrates. This is particularly important in cases involving the adsorption of particles with flexible hairs. We determined that particles with anchored flexible hairs adsorb more strongly to corrugated substrates relative to particles featuring an effective interaction potential shell. The flexibility of the hairs and their ability to adopt a conformation that maximizes the adsorption energy is responsible for increasing the extent of adsorption of such particles relative to their counterparts featuring the effective interaction shell potential. Increasing the length and density of flexible hairs on the particle surfaces further exuberates this effect. Our simulations reveal that it is challenging to decrease the extent of adsorption of spherical particles with flexible hairs on substrates relative to adsorption on flat substrates.

ASSOCIATED CONTENT

Supporting Information
Details pertaining to the computer simulation setup, initialization, operation, and optimization. This material is available free of charge via the Internet at http://pubs.acs.org.

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Notes
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