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#### Oriented-attachment dimensionality build-up via van der Waals interaction

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#### Abstract

In this study, molecular static calculation is carried out to evaluate the van der Waals interaction (vdW) associated with different oriented attachment (OA) growth systems involving 1D nanorods (NRs), 2D nanoplates (NPts) and 3D nanostructures (NSts) for the first time. Our results show that vdW is, to a large extent, determined by the attaching area at all OA growth stages of nanocrystals. vdW increases significantly as the OA growth varies from 1D NR-NP, end-to-end NR-NR assemblies to 2D side-by-side NR-NR /3D NPt-NPt assemblies. Our study reveals the fundamental details in vdW, one of the governing inter-particle interactions involved in OA growth of NCs, and facilitates the analytical understanding of the OA growth thermodynamics.

Keywords: Orientated attachment; Nanocrystal; van der Waals interaction; Molecular static method

#### 1. Introduction

Oriented attachment (OA), uncovered by Peen and Banfield in 1998, is a fundamental growth mechanism for colloidal nanocrystals (NCs).<sup>1</sup> Different from the traditional growth mechanism-Ostwald ripening (OR), OA growth follows "dock and match" process between two precursor nanoparticles (NPs).<sup>2-4</sup> Till now, various nanostructures including 0D nanoparticles (NPs), 1D nanorods (NRs) and 2D nanoplates (NPts) and 3D complex structures, have been synthesized successfully through oriented attachment.<sup>5-9</sup> For instance, the assemblies of NPs along one direction form anisotropic 1D NRs.<sup>10-13</sup> 1D NRs can assemble in either side-by-side or

end-to-end fashion to form 2D NPts or ultra-long nanowires (NWs).<sup>14-16</sup> 2D NPt can further attach with each other to form 3D structures.<sup>17-19</sup>

Despite the synthesis of various structures via OA assembly, the driving force behind these growth deserves our high attention, to understand the thermodynamics and kinetics of OA growth. Recent experimental observations of the early stage of OA assembly of 0D NPs via in-situ high-resolution transmission electron microscopy (HR-TEM) have partly revealed interactions among the approaching NPs, including van der Waals interaction (vdW), Coulombic interactions (CI) and dipolar interactions (DI).<sup>20-22</sup> Theoretical simulations, including molecular dynamic (MD), Monte Carlo (MC) and density functional theory (DFT) calculations have also been carried out to investigate interactions between two 0D NPs in OA growth. For instance, Sathiyanarayanan et al. found that the solvent plays an important role in promoting the anisotropic growth of colloidal Ag nanostructurs.<sup>23</sup> Saidi et al. showed that the surface-sensitive binding of PVP on Ag surfaces origins from the notable difference in vdW attraction on different Ag facets.<sup>24,25</sup> Zhang et al. illustrated the crystallographic orientation-dependent vdW and CI between two nanoparticles either in vacuum or in solution, and they found that vdW is the physical driving force to make two nanoparticle close in the solution since CI is screened.<sup>26,27</sup> However, most of the *in-situ* experiments and simulations focused on OA assemblies between 0D NPs, the investigation of inter-particle interactions in OA growth of NCs with different shapes, varying from 1D NPs, 2D NPts and 3D complex structures is still lacking. The authors have recently studied the CI and vdW between NPs and NRs by constructing a geometrically-spherical NP and a cylindrical NR.<sup>28-31</sup> The CI and vdW contribution between two geometric objects is then given by macroscopic expressions derived via integration over the continuum objects. The vdW interaction between two nanrods assembled either in an end-to-end fashion or a side-by-side fashion was also studied in our previous report.32

The van der Waals interaction between molecules and particles, in air (vacuum) or in liquid, is a fundamental attractive driving force in the OA growth of various nanocrystals with different dimensionalities.<sup>33, 34</sup> Even in some cases, vdW dominates in the assembly of a wide variety of nanostructures.<sup>35-38</sup> Therefore, attentions are mainly focused on vdW in this study. Molecular simulations are employed to resolve vdW between two nanocrystals involving the evolution of the OA growth from 1D NRs to 3D nanostructures. Ag is selected as a materials platform in this study,

but the conclusions in this report are applicable to any materials system. Parameters associated with size and dimensionality of the NCs, and inter-particle separation are explored, which helps to understand the role of the vdW in the OA growth of 1D, 2D and 3D NCs. Special attention is paid to the different OA growth types from NP-NP assembly to NR-NP, NR-NR, NR-NPt, NPt-NPt assemblies. Our study facilitates both the analytical understanding on the evolution of vdW in the growth of all these commonly seen 1D, 2D and 3D OA systems, and the investigation into the fundamental attachment mechanism of an OA system.

#### 2. Models and methods

Four OA growth models are proposed as shown in Figure 1 to demonstrate the NR-NP, end-to-end NR-NR, side-by-side NR-NR and NPt-NPt growths of nanocrystals. In the models, an uncapped NR growth model is chosen to study the vdW. The small NP has several (100) layers stacked in a cubic configuration with cross-section of  $a \times a$ . The large NR also stacks NPs, showing a rectangular configuration, with a length of l and the square cross section of  $a \times a$ . The size range of NPs and NRs in our model lies in 0.4 nm ~12 nm by considering computing complexity and experimental data.<sup>36, 39, 40</sup> The aspect ratio (AR) of the NR can then be defined as l/a and d is the surface-to-surface inter-particle separation between the NR and the NP. Axial NR-NP assembly and end-to-end NR-NR assembly form longer NRs, as shown in Figure 1(a-b). Side-by-side assembly of NRs forms a nanoplate, and NPt-NPt assembly results in larger 3D blocks, as shown in Figure 1(c-d), respectively. Our models are all built along [100] crystalline orientation. NP and NR models along [110] and [111] orientations are also built. The facet effect on vdW is investigated as shown in Figure S1 in the supporting information. In this work, to investigate the dimensionality effect, the facet effect is eliminated by fixing the assembly orientation to [100]. The three orientations of [100], [010] and [001] are equivalent for face-centered cubic metals like Ag, which can eliminate the effect crystalline orientation on vdW and facilitates the investigation of the OA assembly of Ag NCs in 2D or 3D fashions. In addition, simple cubic geometric shapes are used rather than the thermodynamically stable Wuff' structure. This is because that most synthetic experiments are carried out under the kinetic control, thermodynamical equilibrium is difficult to reach. The addition of surfactants or other additives in solutions also alters the shape. For instance, rectangular Ag nanorods were successfully synthesized in polyol and PVP environment.<sup>40</sup> Cubic Ag models were also employed in the 3 simulation work of Sathiyanarayanan et al.<sup>23</sup>



Figure 1. The sketches of the OA growth models: (a) 1D NR-NP, (b) 1D NR-NR of end-to-end, (c) 2D NR-NR of side-by-side and (d) 3D NPt-NPt assembly. A nanocube with an edge length of *a* stands for a NP. A NR has a cross-section of  $a \times a$  and a length of *l*. *d* is the surface-to-surface inter-particle separation between two NCs. In (c), side-by-side assembly of NRs forms a nanoplate. In (d) NPt-NPt assembly results in larger 3D blocks.

The universal force field (UFF) was used to calculate the vdW by molecular static simulation,<sup>41</sup> and the vdW is defined by the Lennard-Jones potential given in Eq.1.<sup>42,43</sup>

$$E = D_0 \left[ \left( \frac{r_0}{r} \right)^{12} - 2 \left( \frac{r_0}{r} \right)^6 \right]$$
 Eq. 1

where  $r_0$  is the equilibrium bond distance, r is the atomic separation, and  $D_0$  is the depth of equilibrium potential well. The Lennard-Jones potential is a relatively compromised approximation since more accurate calculation methods such as DFT require excessive computing resources in the large 2D/3D models of this work. The vdW between any two atoms is summed without truncation. As the atoms on the two surfaces form chemical bonds, the inter-planar distance is the zero separation between NR and NP (d = 0). Although the vdW is much weaker than the chemical bond, the vdW is the attractive driving force for two particles approaching together and thus cannot be neglected. The total vdW for the configuration of the NR and NP with a separation of *d* is calculated as  $E_{vdw}(d)$ , which contains the vdW between any two atoms in the NP and the NR. The vdW with an infinite inter-particle separation is calculated as  $E_{vdw}(\infty)$ , which eliminates the vdW between one atom from the NP and another atom from the NR ( in our work,

 $E_{vdw}(d)$  varies little at adequately large *d* and can be used to substitute  $E_{vdw}(\infty)$ ). Then, the vdW energy between the NP and the NR with a separation distance of d ( $\Delta E_{vdw}(d)$ ), which is the summed vdW between atom pairs with one atom in the NP and another atom in the other NP or NR, can be calculated by the difference of  $E_{vdw}(d)$  and  $E_{vdw}(\infty)$ , as given by Eq.2,

$$\Delta E_{vdw}(d) = E_{vdw}(d) - E_{vdw}(\infty) \qquad \qquad Eq. 2$$

It should be noted that parameters in a real synthetic environment of OA growth, such as temperature, solvent and ligands are not considered in this simulation since these parameters only affect the quantitative value of vdW; the main conclusions in this study are not influenced without considering these parameters.

#### 3. Results and discussions

In OA growth of NRs, NPs may approach NRs from all directions. NPs approach along the NR axial direction, which leads to the elongation of NRs, and NPs can also attach NRs from the sides of the NR. To compare the magnitudes of the vdW interactions in the two attachments, four approaching patterns are designed including (a) axial direction, (b) 0*l* top side (0*l*), (c) 0.25*l* side, and (d) 0.5*l* side attachments, respectively. Fixing *a* at 1.2 nm, the vdW for above four approaching patterns is calculated, as shown in Figure 2. The critical points ( $d_c$ ) of vdW *versus d* plots, at which vdW begins to be smaller than 0.1 Kcal/mol, are similar for the four cases, with variations less than 0.05 nm. The inset in Figure 2 shows vdW at zero separation between the NP and the NR ( $\Delta E_{vdw}(0)$ ) for different types of NR-NP systems. The result indicates that  $\Delta E_{vdw}(0)$  for the NP sideway attaching at the middle of the NR (0.25*l* ~0.5*l*) has the most negative value, which suggests that the sideway growth is thermodynamically favored for a NR growth *via* OA. Therefore in order to obtain axial growth, appropriate ligands should be used during the synthesis of nanoparticles to selectively passivate the side surfaces of NR and suppress the sideway growth.



**Figure 2.** Plots of vdW *versus* NR-NP separation when NPs approach the side of a NR from four different directions: (a) axial approach, (b) top side (0*l*), (c) 0.25*l*, and (d) 0.5*l*. Both NR and NP are fixed with *a* of 1.2 nm and the NR is fixed with an AR of 10. Inset:  $\Delta E_{vdw}(0)$ *versus* the attaching site on the side of a NR.

The effect of the diameter of the NR and NP on the vdW in the axial NR-NP assembly is investigated. Figure 3 illustrates the interaction of the NP and NR with *a* from 0.4 nm to 4.2 nm with a fixed AR of the NRs at 10. The vdW between the NR and the NP decreases as the separation *d* increases. As vdW approaches ~0.1 Kcal/mol, inflection features appear in the plots of Figure 3, and vdW decreases rapidly to zero above these features. The critical separations for the NPs and NRs with the diameters of 0.4 nm, 0.8 nm, 1.2 nm, 2.5 nm and 4 nm are 0.2 nm, 0.4 nm, 0.6 nm, 1.2 nm and 1.9 nm, respectively. *d<sub>c</sub>* is nearly proportional to *a*. The attaching energies,  $\Delta E_{vdw}(0)$ , for the OA growth of NRs with the above diameters are -0. 54 Kcal/mol, -2.09 Kcal/mol, -4.71 Kcal/mol, -19.04 Kcal/mol and -53.35 Kcal/mol, respectively, indicating that there is a much larger vdW for the OA growth of NR with larger diameters. This implies that NRs and NPs with larger diameters are more likely to attach if the attachment is mainly governed by the van der Waals interaction.



Figure 3. Plots of vdW *versus* NR-NP separation for NR and NP with different diameters and an AR = 10. The dotted lines indicate the critical separations.

The plots of vdW *versus* separation *d* are shown in Figure 4, which involve the elongation of NRs *via* 1D axial NR-NP assembly (Figure 4a) and *via* 1D end-to-end NR-NR assembly (Figure 4b), the growth of NPts *via* 2D side-by-side NR-NR assembly (Figure 4c) and the growth of 3D NSts *via* 3D NPt-NPt assembly (Figure 4d). As shown in Figure 4a-b, the overlap of the curves of vdW *versus d* indicates that the elongation of the NRs (the increase in AR), either by axial NR-NP or end-to-end NR-NR assemblies, does not affect vdW between the two approaching NPs or NRs. The critical distance at which vdW goes below -0.1 Kcal/mol is approximately 0.6 nm in both

assembly fashion. The vdW attachment energy at the zero separation in the end-to-end NR-NR assembly is about ~-4.99 Kcal/mol, which is slightly larger than ~-4.89 Kcal/mol in the axial NR-NP model. This result implies that the above two ways of assembly experiences a similar energy barrier, and thus either the NR-NP model or the end -to-end NR-NR model is possible in the OA growth of 1D NRs as considered from an energy point of view of vdW.

The curves of vdW versus *d* also overlap either in the side-by-side growth of NRs to NPts or in the NPt-NPt assembly to 3D nanostructures as shown in Figure 4c-d, which indicates that the vdW changes little as ARs change at all stages of the OA growth of nanocrystals as the attaching areas remain unchanged. The critical distance,  $d_c$ , during the whole side-by-side growth of the NRs varies little ~1.3 nm.  $\Delta E_{vdW}(0)$  also holds a constant value of -27.2 Kcal/mol. In the OA growth of 3D nanostructures *via* NPt-NPt assembly,  $d_c$  and  $\Delta E_{vdW}(0)$  are 2.7 nm and -154.3 Kcal/mol, respectively. These data along with the data of  $d_c$  and  $\Delta E_{vdW}(0)$  in the end-to-end NR-NR assembly `demonstrate that both  $d_c$  and  $\Delta E_{vdW}(0)$  increase significantly as the growth model varies from 1D end-to-end NR-NR/2D side-by-side NR-NR, to 3D NPt-NPt. Such a trend can be illustrated by the fact that the three growth patterns have different contact areas, which are 1.44 nm<sup>2</sup>, 7.2 nm<sup>2</sup> to 36.0 nm<sup>2</sup>, and only the atoms adjacent to the OA coalescence interface contribute to the major portion of vdW. Therefore, in the OA assembly, the inter-particle vdW increases as the attaching area increases if surface states at different sites of the assembled nanostructures, such as polarization and surface ligands, are identical.



**Figure 4.** Plots of vdW *versus* separation d with fixed *a* value 1.2 nm. The red vertical dash line indicates the location of the critical distance at which the vdW energy is 0.1 Kcal/mol. (a) 1D NR formation by NR-NP model with NRs of different ARs, (b) 1D NR formation by NR-NR end-to-end model with one of the NR of different length. Two primary NRs attach each other form a 2NR (NR-NR) in an end-to-end fashion. A 2NR and a primary NR form a 3NR (2NR-NR). A 3NR attaches a NR, forming a 4NR.(3NR-NR), a 4NR can further attach more NRs. Two 2NRs can also attach each other to form a 4NR (2NR-2NR). (c) 2D NPt formation by NR-NR side-by-side model. 2NR, 3NR and 4NR are formed in the side-by-side fashion. (d) 3D nanostructure formation by NPt-NPt model. 2NPt, 3NPt and 4NPt are formed via face-to-face assemblies of two, three and four NPts, respectively.

In this report, we investigated the vdW variation in OA growth by constructing experimental-observable assembly models of different dimensions. Our study facilitates the understanding of OA growth thermodynamics from an energy point of view. However, the other inter-particle interactions, such as Coulumbic interaction and dipolar interaction are not included. The accurate calculation of vdW by involving the effects of surface ligands and solvents in the OA growth are also unexplored in this study. All of these factors will be a focus of our future study.

#### 4. Conclusion

In summary, the vdW in the OA growth of 1D NRs, 2D NPts and 3D nano-structures were studied by the molecular static calculation. It has been found: (1) in the 1D NR-NP assembly, NPs assemble more easily at the sideway of NRs than at the axial direction, and thus appropriate ligands must be used in the synthesis to selectively passivate the side planes of NRs and suppress the sideway growth; (2) in the axial NR-NP and NR-NR end-to-end assembly, the growth of 1D NRs is only sensitive to the diameter of the NRs rather than the AR of NRs; (3) as OA growth varies from end-to-end NR-NR to side-by-side NR-NR/NPt-NPt assemblies, an increased vdW is

experienced due to the increased attaching area. Our calculations improve the analytical understanding on the correlation between the evolution of vdW and the 1D, 2D and 3D OA assemblies at various growth stages.

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### Table of content:

Molecular static calculation is carried out to evaluate the role of van der Waals interaction associated with different oriented attachment growth systems involving 0D nanoparticles, 1D nanorods, 2D nanoplates and 3D nanostrucutres.

## **Graphical abstract:**

