# Supplemental material for "Collective Effect on Thermophoresis of Colloids: a Microfluidic Study within Framework of DLVO Theory"

Yugang Zhao, Cunlu Zhao, Jinhua He and Yi Zhou and Chun Yang*

School of Mechanical and Aerospace Engineering, Nanyang Technological University

50 Nanyang Avenue, Singapore 639798

*To whom the correspondence should be addressed. Tel: +65-6790-4883; Email: mcyang@ntu.edu.sg.

## S1 Details of 3D-lattice model for particle interaction

In order to evaluate Eq.(5) in the manuscript, we first need to know the spatial arrangement of particles in the solution. Here, it is assumed that the particles in the space form a 3D lattice structure as detailed in Figure S1. Actually, this concept is not completely new. Van Megen and Snook[1] showed that the particle suspensions can form ordered lattice structures. In addition, the lattice concept was also used for modeling the structure of charged colloidal particles[2]. Similar to our situation, Luettmer-Strathmann[3] adopted the lattice concept to calculate the interaction energy between a polymer chain and its surrounding solvent molecules. However, they only considered the interactions due to nearest surrounding solvent molecules. In our case a particle interacting with all its neighboring particles is taken into account. To calculate the total interaction energy on one particle, we must add up the interaction energy due to all the surrounding particles, rather than just the nearest surrounding particles. Figure S1 schematically shows the steps used for calculating the total interaction energy on one particle (located in the origin with shown in the red color). First, we calculate the interaction energy between the red particle (at the origin) and every single particle in each layer (Figure S1 (a), (b), (c) and (d)). Then, summing up the obtained interaction energy, we get the interaction energy on the red particle (at the origin) due to each single layers. Finally, the total interaction energy on the red particle can be obtained by summing the interaction

energy due to single layers. In the calculations, the distribution of particles is assumed to be locally homogeneous, with the shortest interparticle distance being $h$+2$a$ (wherein $h$ is the particle surface-surface distance, and $a$ is the particle radius). With the aforementioned procedures, the total interaction energy on the red particle (or Eq.(5)) can be obtained as

$$\begin{aligned}\psi(h) = \sum_{i=1}^{\infty}\Big[6\phi\big(i(h+2a)-2a\big)+12\phi\big(\sqrt{2}i(h+2a)-2a\big)+8\phi\big(\sqrt{3}i(h+2a)-2a\big)\Big] \\ +24\sum_{i=2}^{\infty}\sum_{p=1}^{i-1}\Big[\phi\big(\sqrt{i^2+p^2}\,(h+2a)-2a\big)\Big] \\ +24\sum_{i=2}^{\infty}\sum_{p=1}^{i-1}\Big[\phi\big(\sqrt{2p^2+i^2}\,(h+2a)-2a\big)+\phi\big(\sqrt{2i^2+p^2}\,(h+2a)-2a\big)\Big] \\ +48\sum_{i=3}^{\infty}\sum_{p=2}^{i-1}\sum_{q=1}^{p-1}\phi\big(\sqrt{i^2+p^2+q^2}\,(h+2a)-2a\big)\end{aligned} \tag{s1}$$

where the first term corresponds to the contribution due to black particles in the lattice shown in Figure S1, the second term corresponds to the contribution from the blue particles in the lattice shown in Figure S1, the third term corresponds to the contribution from the pink particles in the lattice shown in Figure S1, and the fourth term corresponds to the contribution from the green particles in the lattice shown in Figure S1. It should be noted that Eq.(s1) is an equivalent form of Eq.(6) in the manuscript.

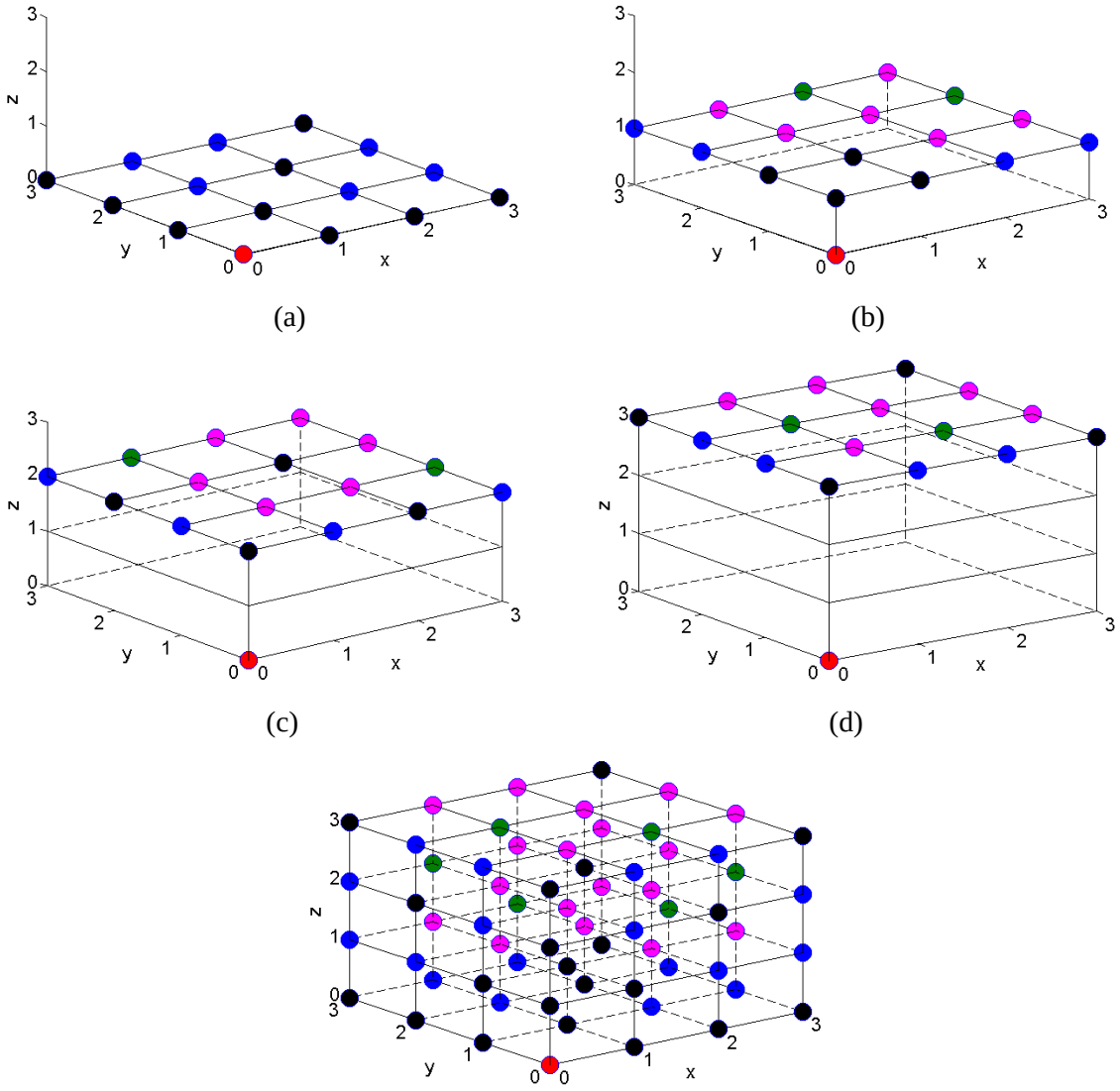


Figure S1 3D-lattice model for calculation of the total interaction energy on a single particle. Specifically, the total interaction energy on the red particle at the coordinate (0, 0, 0) is calculated. (a) The particles which interact with the red particle are distributed at the nodes of lattice in the first layer; (b) The particles which interact with the red particle are distributed at the nodes of lattice in the second layer; (c) The particles which interact with the red particle are distributed at the nodes of lattice in the third layer; (d) The particles which interact with the red particle are distributed at the nodes of lattice in the fourth layer; (e) The superposition of (a) to (d) forms a 3D particle lattice structure. The black particles correspond to the first term of Eq.(s1), the blue particles represent the second term of Eq.(s1), the pink particles denote the third term of Eq.(s1), and the green particles represent the last term of Eq.(s1). One unit in all three coordinates has a dimension of (h+2a).

## References

1. W. Van Megen and I. A. N. Snook, *Nature*, 1976, **262**, 571-572.
2. S. N. Petris, J. Stankovich, D. Y. C. Chan and R. H. Ottewill, *Langmuir*, 2003, **19**, 1121-1126.
3. J. Luettmer-Strathmann, *The Journal of Chemical Physics*, 2003, **119**, 2892-2902.