NanoDiaRA

Understanding the colloidal behavior of nanosized iron oxide particles in complex biological environment

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Project Goals / Objectives

In the aim of using nanoparticles for biomedical applications, especially superparamagnetic iron oxide nanoparticles (SPION), it is crucial to be able to predict well the colloidal stability of the SPION suspension starting from synthesis, functionalization until its end-use in a living body, as aggregation of SPION will strongly affect the outcome of experiments, by e.g. changing the yield of coating and functionalization of the surface, enhancing dramatically the immunological response of the organism, by modifying the magnetic properties of the SPION, etc…

Our final goal is to develop a comprehensive tool to predict at least qualitatively the colloidal behavior of SPION as well in simple colloidal systems as in complex media such as blood serum or synovial liquid. This will allow us to determine what type of interactions between the particles and biomolecules are possible from a physical point of view, thus helping to interpret and discuss the outcome of molecular "fishing" experiments.

Theoretical Approach

A classical way to predict particle-particle interactions in a suspension is done by use of the Derjaguin-Landau and Verwey-Overbeek (DLVO) theory [1] [2]. This theory has been repeatedly shown to predict with good agreement with experiments the forces of interactions for particles typically above 100nm in simple, dilute solutions ($c_{ionic} \approx 10^{-2}$ M).

Inspired from Velegol's [3] work (among others), we propose for the case of this project to investigate the suitability of an **well adapted, extended DLVO theory** as follow:

$$\Phi_{DLVO} = \Phi_{vdW} + \Phi_{es}$$

vdW interact. / elect. interact.
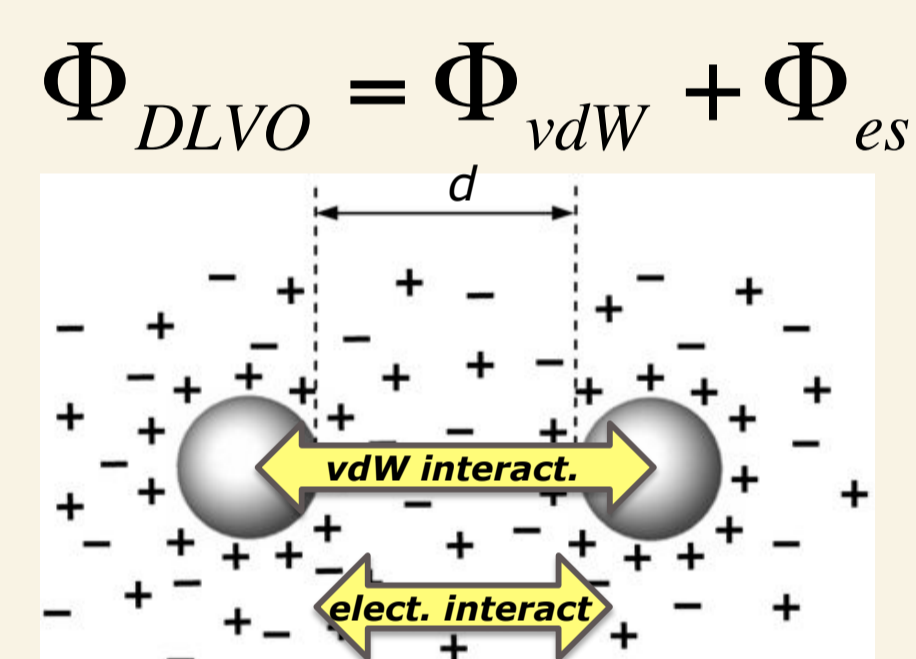
$$\Phi_{X-DLVO} = \Phi_{wdV} + \Phi_{es} + \Phi_{dep} + \Phi_{steric} + \Phi_{bio} + \Phi_{magn}$$

Based on this simple equation, we wish to bring understanding whether the physical models describing the different potentials
- are relevant / dominant in our particle system,
- are developed from assumptions (physically "valid") for both nanosized particles *and* complex suspending media
- are in good agreement with experimental results

Open questions - Outlook

- Most models take into assumptions particles with diameters

  What happens when particles have size similar to ionic double layer or biomolecule?

- Need to verifiy interaction by elaborate computer simulations
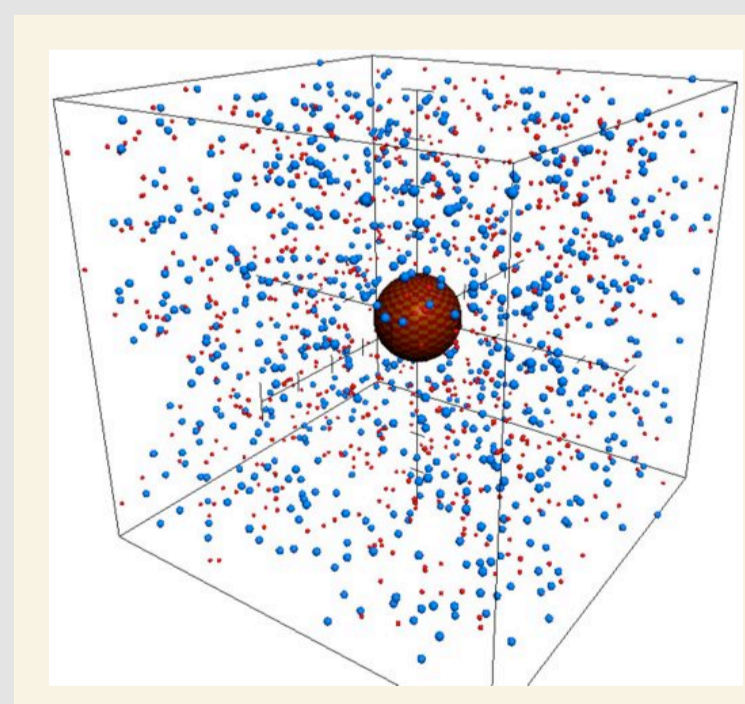
- Biological media complexity:
  - high complex ionic strength
  - complex macromolecules

  Can biomacromolecules be viewed as particles?

Particle interaction potentials

### Φ_{vdW} London-van der Waals interaction

Coupling of the spontaneous momentary dipolar of moments of the particles, that results in an always attractive interaction. For very small particles or long distances, retardation effects appear due to the finite velocity of light. The London-van der Waals interaction is mainly responsible for the non-reversibility of the aggregation mechanism. Classically, the interaction potential is being described by [4]:

$$\Phi_{vdW} = -\frac{A_H}{6}\left[\frac{2R_1R_2}{C^2-(R_1+R_2)^2} + \frac{2R_1R_2}{C^2-(R_1-R_2)^2} + \ln\frac{C^2-(R_1+R_2)^2}{C^2-(R_1-R_2)^2}\right]$$

### Φ_{es} Electrostatic interaction

Coulombic repulsion between two same sign charged particles. The importance of this potential for the colloidal behavior depends strongly upon the ionic strength of the media, as ions co-interact and screen the charge effect. Can be described by [5]:

$$\Phi_{es} = \pi\varepsilon\varepsilon_0\frac{R_1R_2}{R_1+R_2}\left[(\psi_1+\psi_2)^2\ln\left(1+e^{-\kappa d}\right) + (\psi_1-\psi_2)^2\ln\left(1-e^{-\kappa d}\right)\right]$$
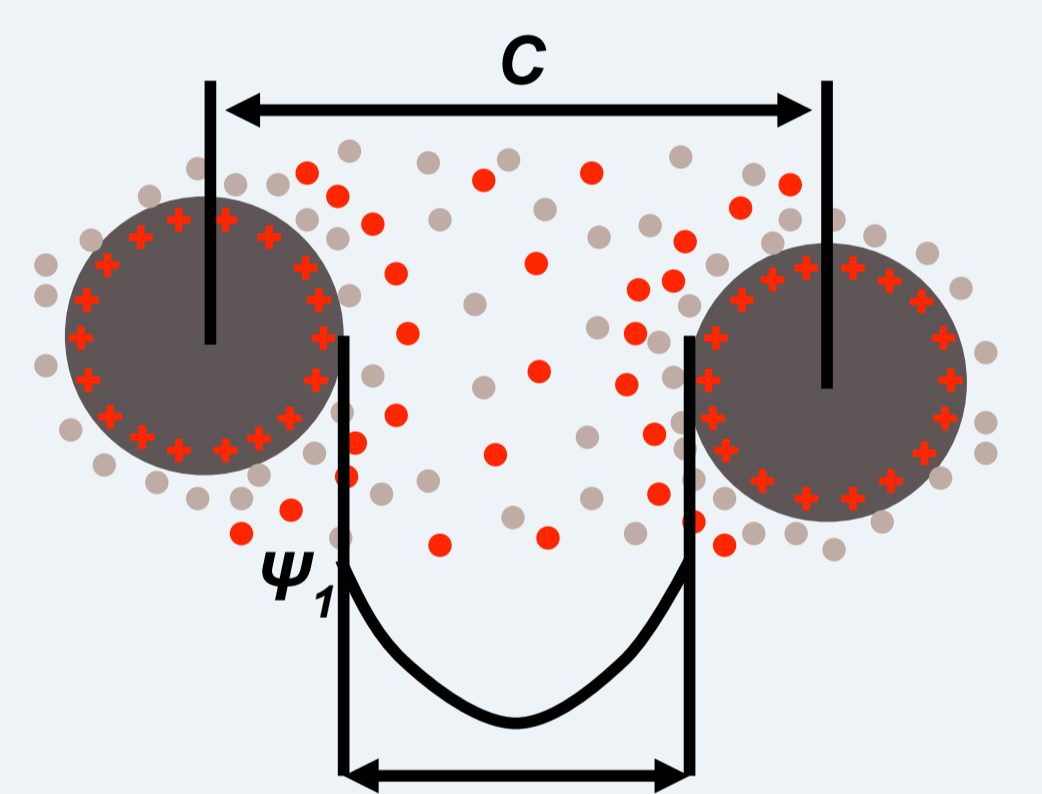
Φ_{dep} Depletion interaction

Forces resulting from osmotic pressure, which arise in presence of solvent molecules. When the distance between particles is small in comparison with the molecule size, excluded volumes with lower concentrations appear in the middle, which result in an osmotic pressure / force.
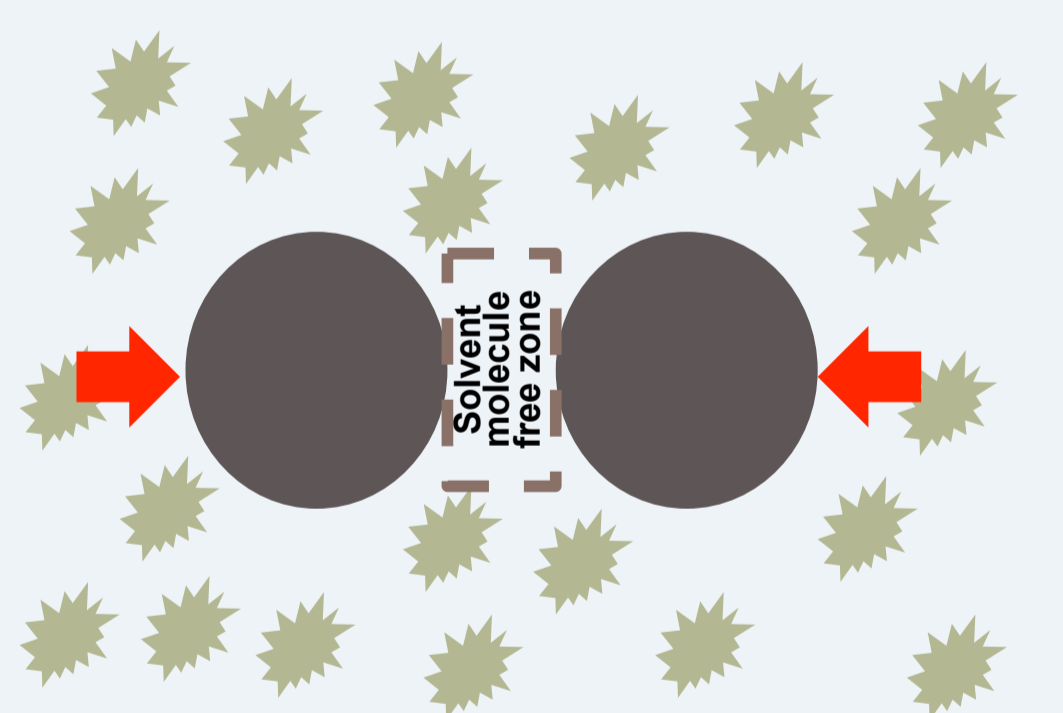
Φ_{steric} Steric interaction

When a polymer or soft biomolecule is coating the particles surfaces, it can act as a steric barrier that will prevent the particles surfaces from getting very close, thus preventing strong vdW interactions to arise.

Φ_{bio} Biological interaction

Very complex interactions arise between particles and complex biofluids (especially complex biomolecules). We propose to break up the complexity by considering the molecules as particles and using:

$$\Phi_{Bio} = \Phi_{Bio,wdV} + \Phi_{Bio,es} + \Phi_{Bio,steric}$$

Φ_{magn} Magnetic interaction

Attractive magnetic dipole-dipole interactions arise between the particles when put into a magnetic field. To that, a van der Waals like interaction appears between oscillating magnetic fields [6].

References

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