DLVO theory of colloidal aggregation

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Fundamentals of DLVO theory

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Landau
Verwey
Overbeek

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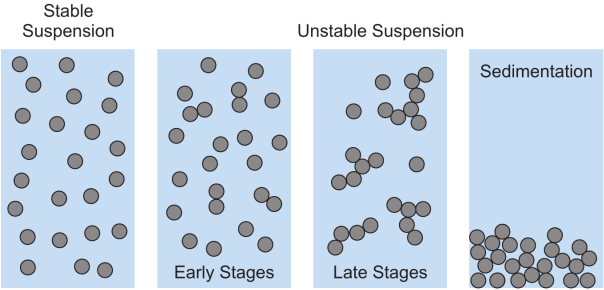

Credit: Trefalt and Borkovec

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Fundamentals of DLVO theory

Online resources are available from Github (slides and codes):
https://github.com/mcaroba/dlvo

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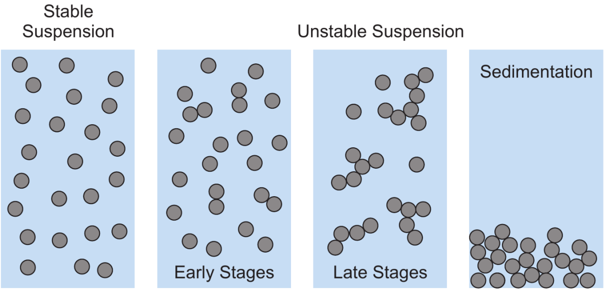

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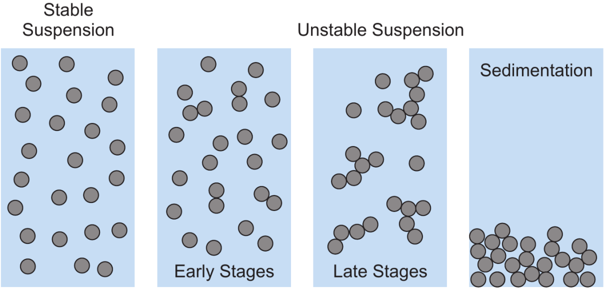

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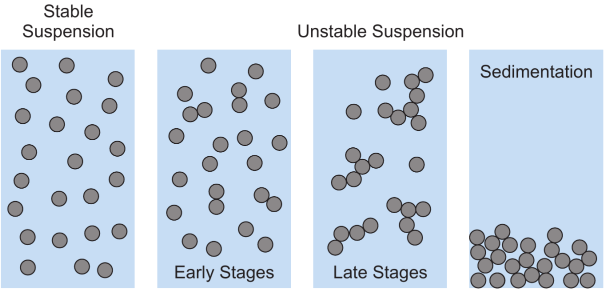

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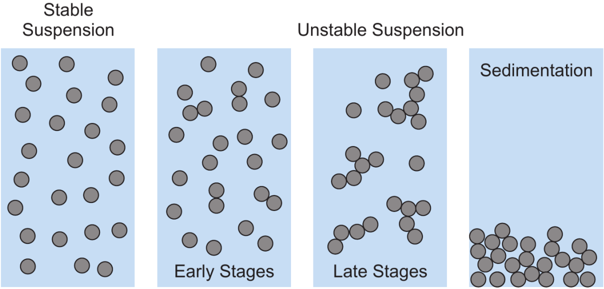

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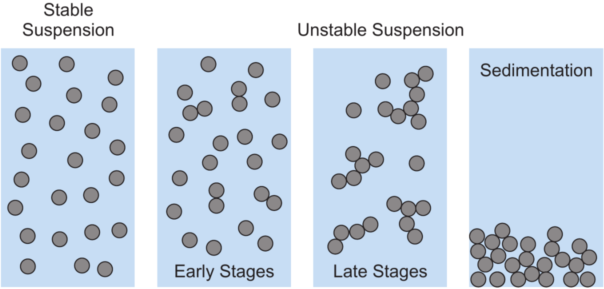

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- Question 2: for how long does it remain stable (long enough for our experiment?)

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h is the separation between the surfaces ($\neq d$); κ is the inverse Debye length; H is Hamaker's constant[1]; W is energy per surface area.

[1]Originally called A in H. C. Hamaker, Physica 4, 1058 (1937).

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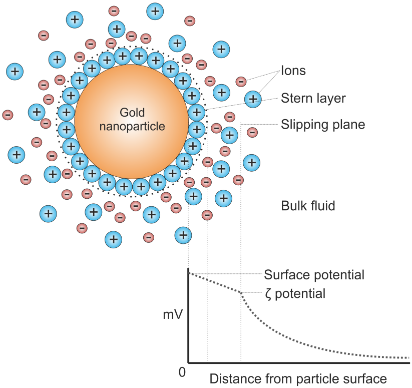
The electrical double layer:



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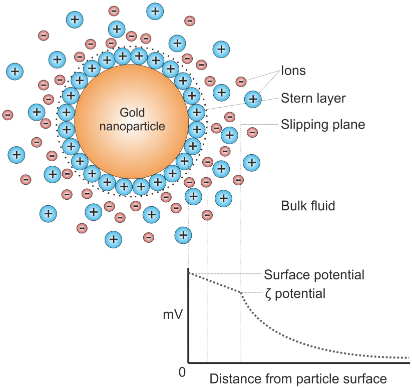

Due to the EDL the electrostatic potential is screened out. The Debye lenght $1/\kappa$ gives the typical distance over which the decay is significant.

$$W_{\mathrm{EDL}}(h) = \frac{2\sigma_1\sigma_2}{\varepsilon\varepsilon_0\kappa}\exp(-\kappa h) \quad (5)$$

$$\kappa = \sqrt{\frac{2e^2 N_{\mathrm{A}} I}{k_{\mathrm{B}} T \varepsilon\varepsilon_0}} \quad (6)$$

$$I = \frac{1}{2}\sum_i z_i^2 c_i \quad (7)$$

I is the ionic strength of the solution and c_i the concentration of each ion type with charge z_i (units of e)

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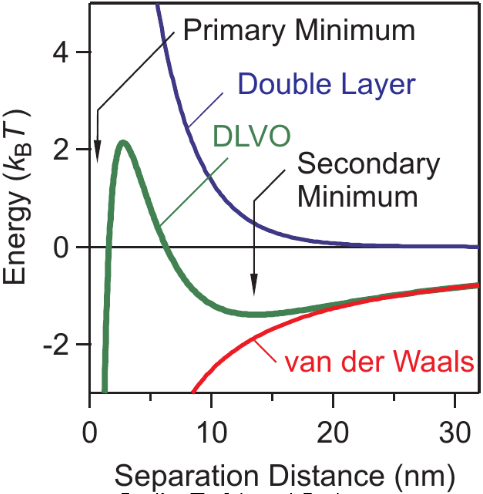
Strength of the DLVO interaction determines aggregation behavior:



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Fundamentals of DLVO theory

A computational experiment:

(8)

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`https://github.com/mcaroba/dlvo`

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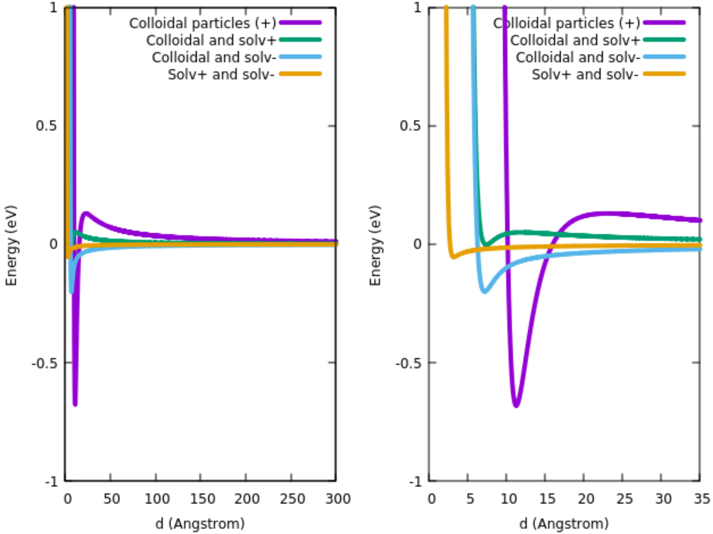
Our individual interactions look like this:



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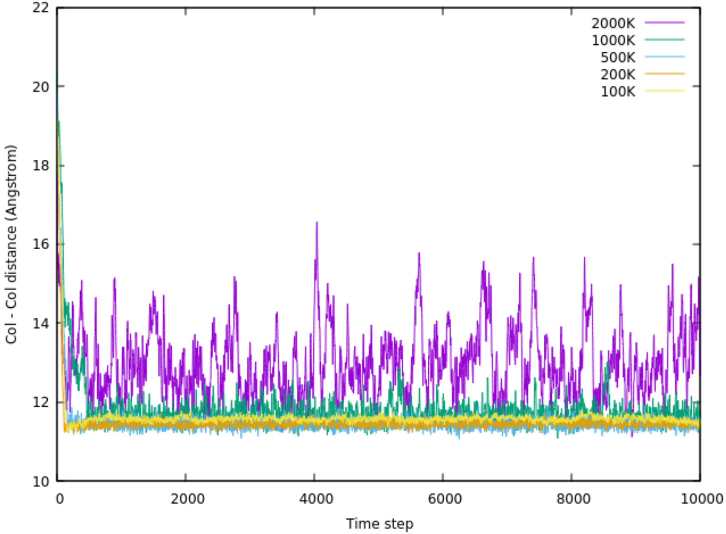
The stability of the suspension depends on the temperature:



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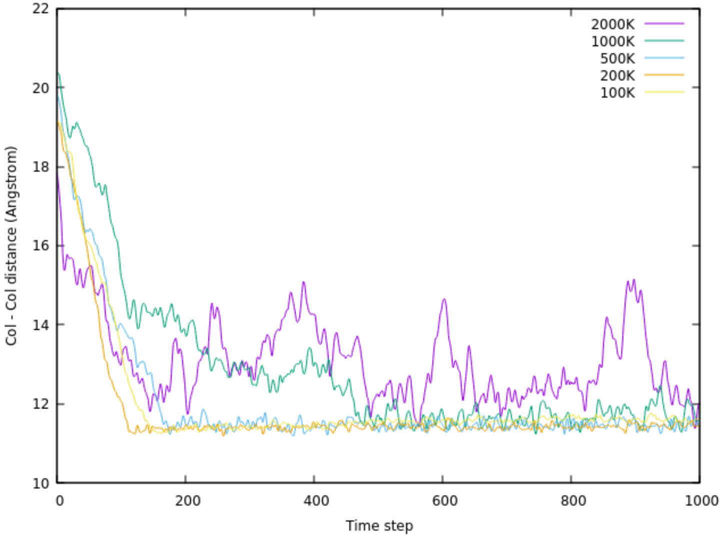

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DLVO theory predicts the following expression for the aggregation rate:

$$k = \frac{2k_\mathrm{B}T}{3\eta R_\mathrm{eff}} \left(\int_0^\infty \mathrm{d}h \frac{1 + R_\mathrm{eff}/h}{(R_1 + R_2 + h)^2} \exp\left(U(h)/(k_\mathrm{B}T) \right) \right)^{-1} \qquad (10)$$

where $U(h)$ is the energy of the interaction between the colloidal particles according to the DLVO approximation, R_eff is the reduced radius ($R/2$ for idential particles) and η is the viscosity of the solvent.

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By fine tuning the simulation parameters we can try to estimate this coefficient from the computational experiment and compare to the value obtained analytically by DLVO. Possible project assignment topic!