SCEJ 90th Annual Meeting
Mar. 13, 2025

Particle distribution and conductivity in nanocomposite coatings: Effects of interactions between different particle species

ナノコンポジット塗膜内の粒子分布と導電性：異種粒子間相互作用の影響

○ 辰巳 怜 （PIA）
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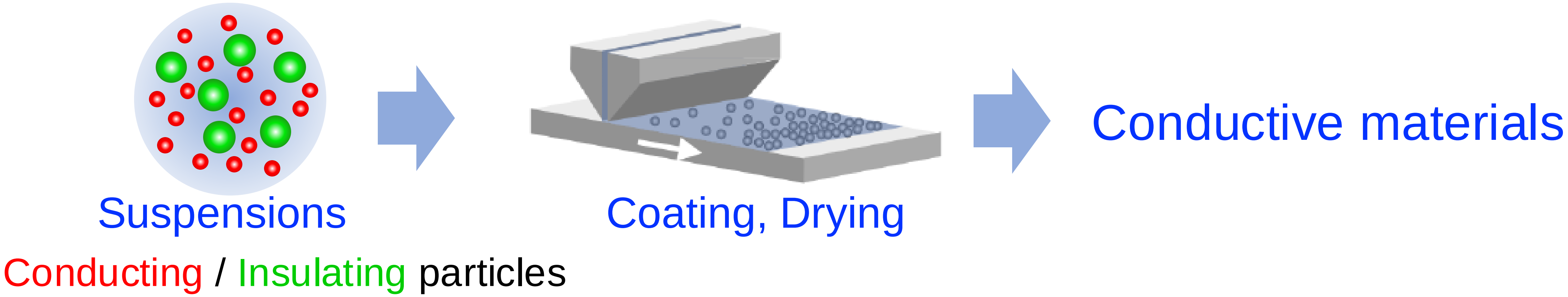
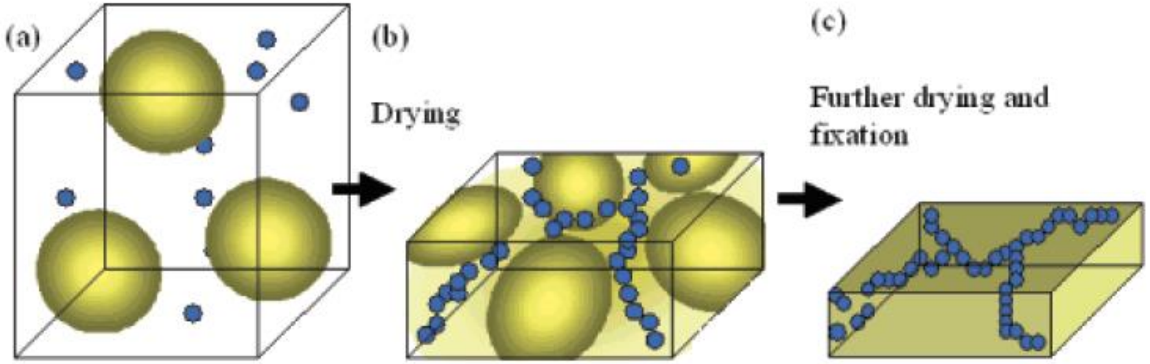
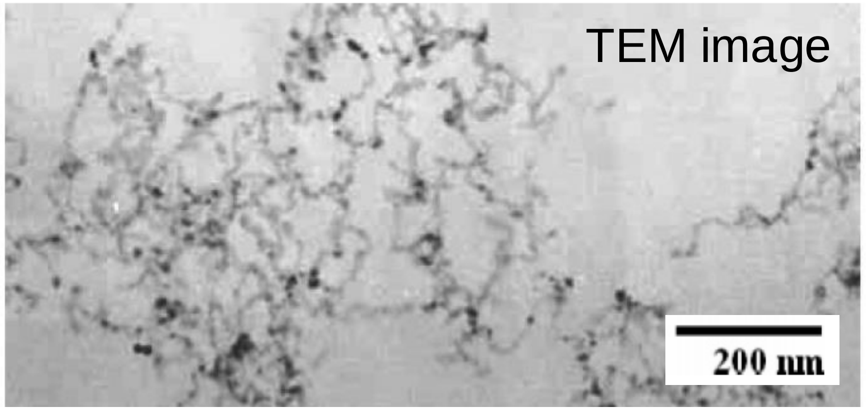
吉江 建一 （PIA）
辻 佳子 （東大環安セ/東大院工）



Conductive nanocomposite coatings

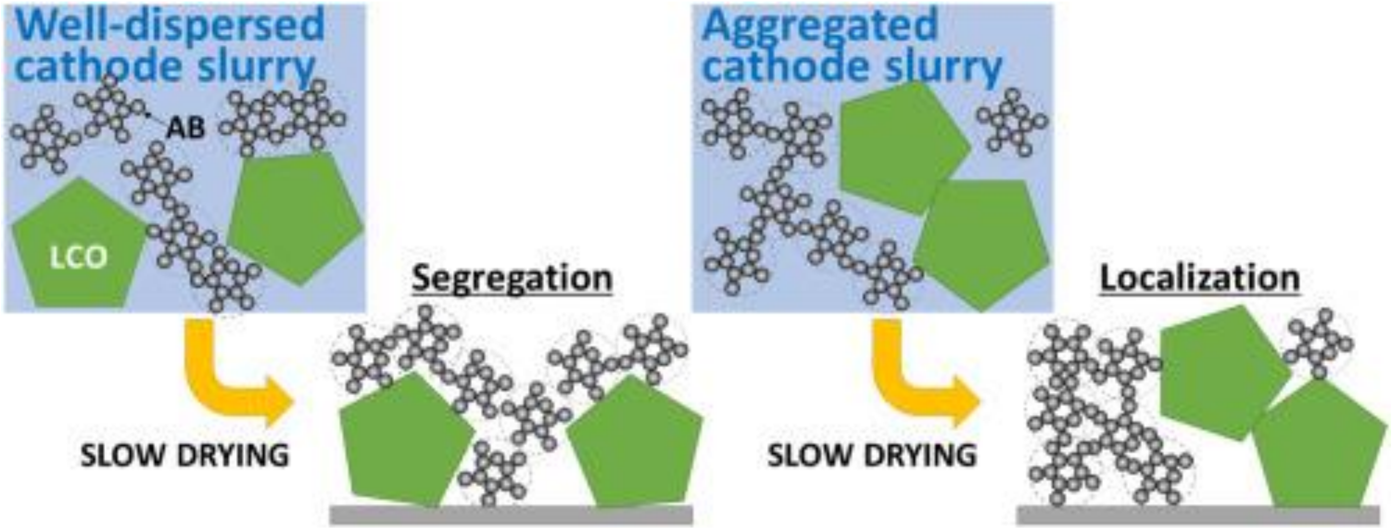
Transparent conductive films (Latex + ATO)

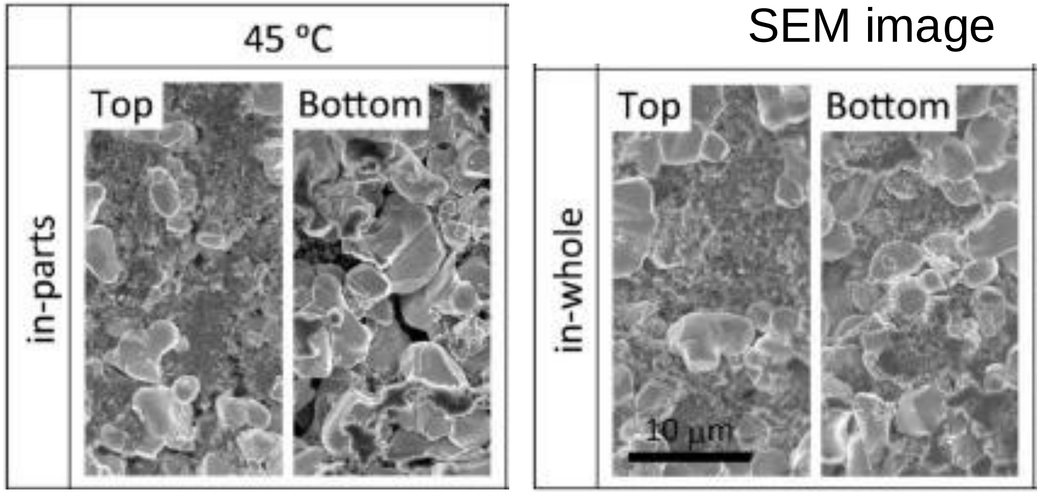




Wakabayashi *et al*., Langmuir **23**, 7990 (2007).

Battery electrode (LCO + AB)

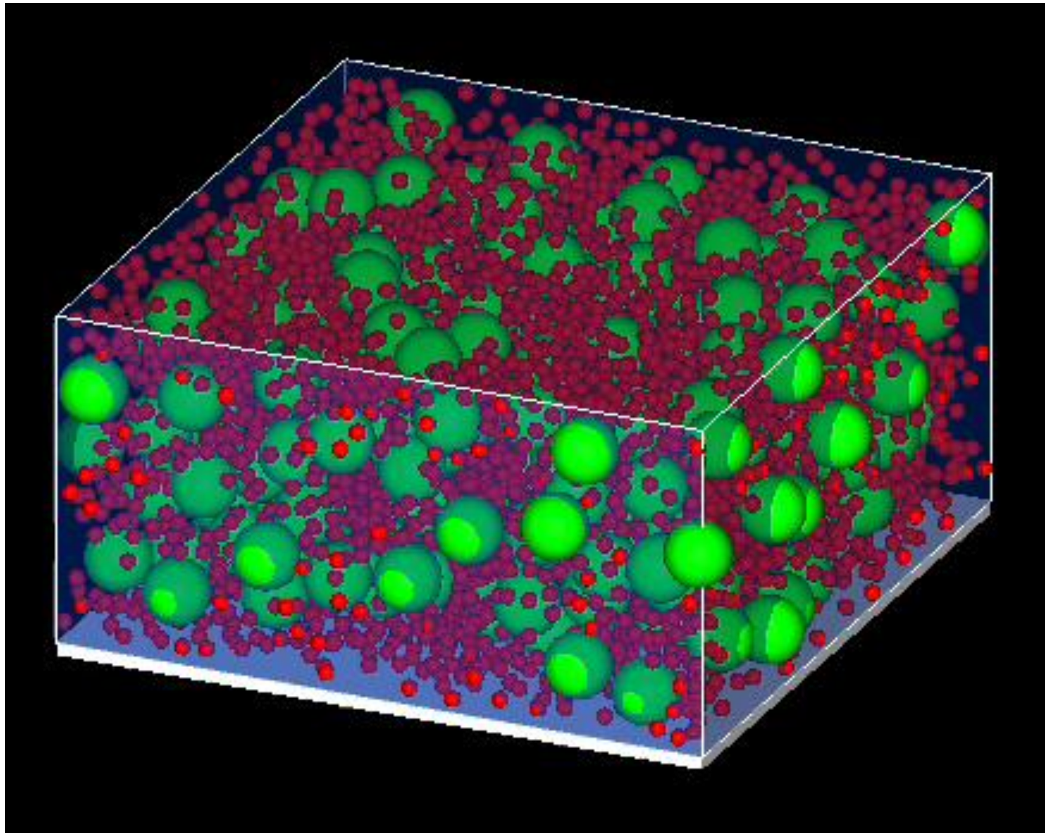


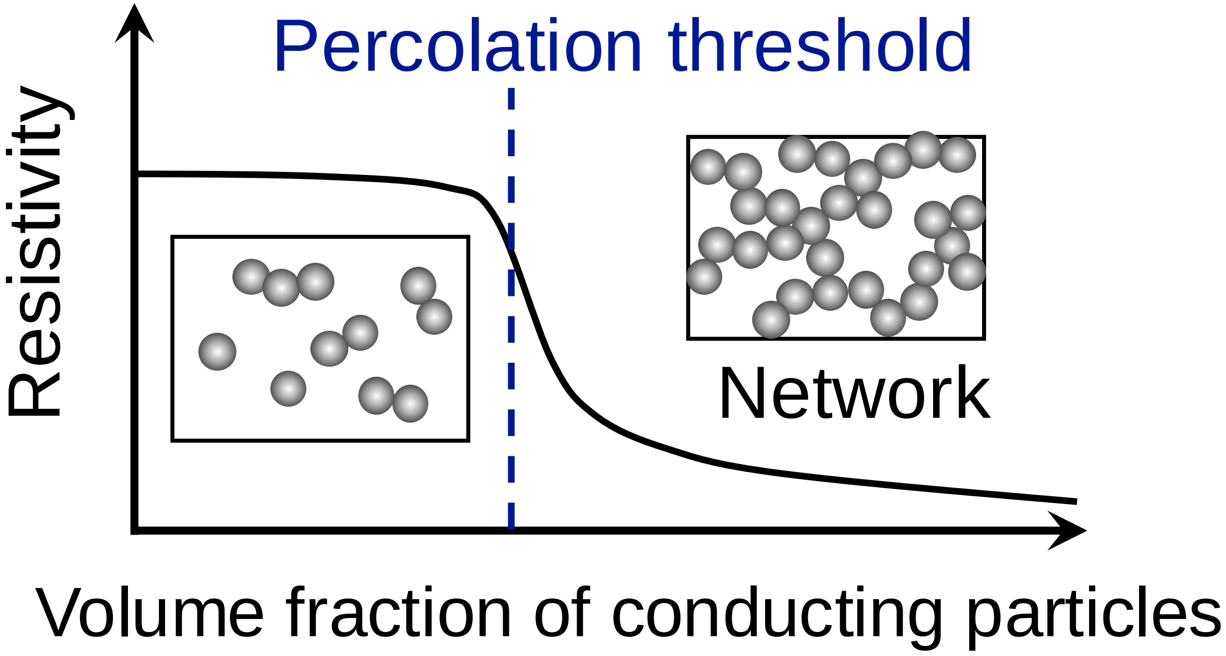


Komoda *et al*., J. Power Sources **568**, 232983 (2023).

Previous study: Numerical simulation

Drying of colloidal mixture (**Conducting** / **Insulating** particles)

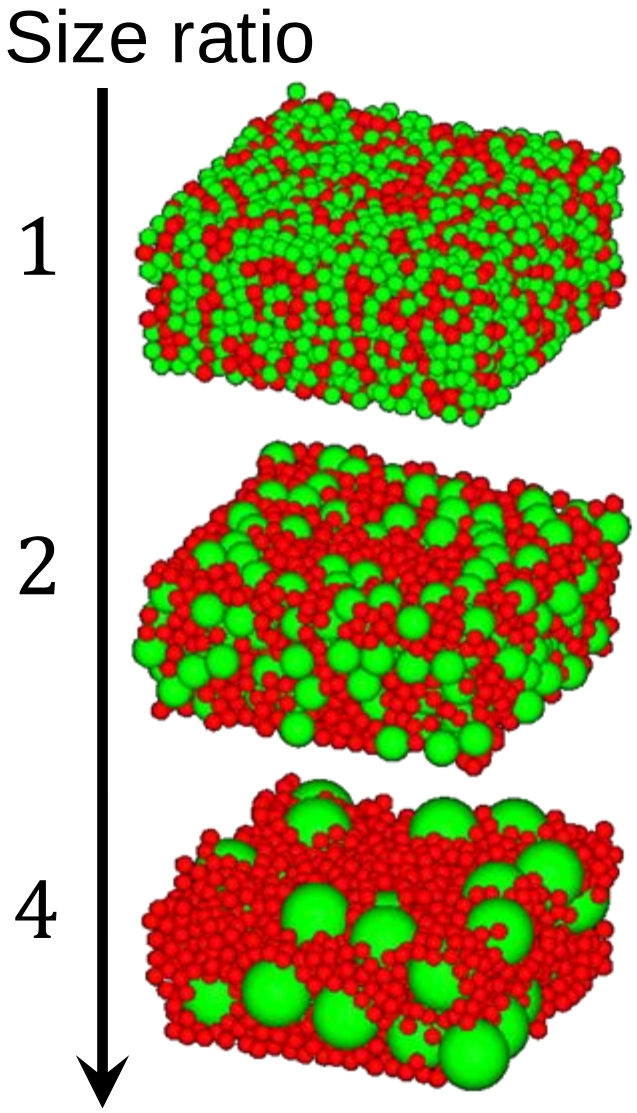




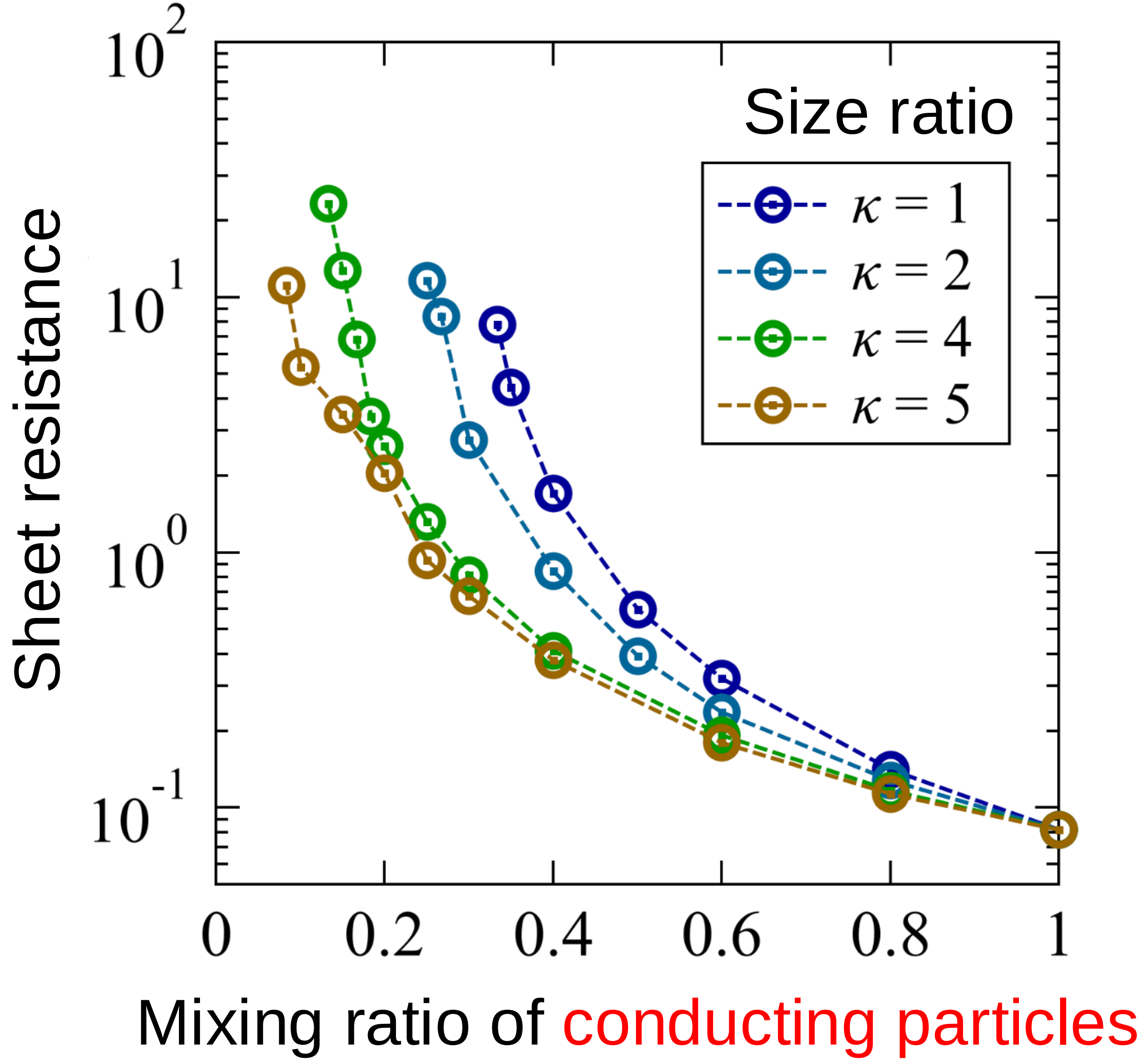
Particle size ratio → Conducting network → Conductivity

Tatsumi *et al*., SCEJ 52nd Autumn Meeting (2021).

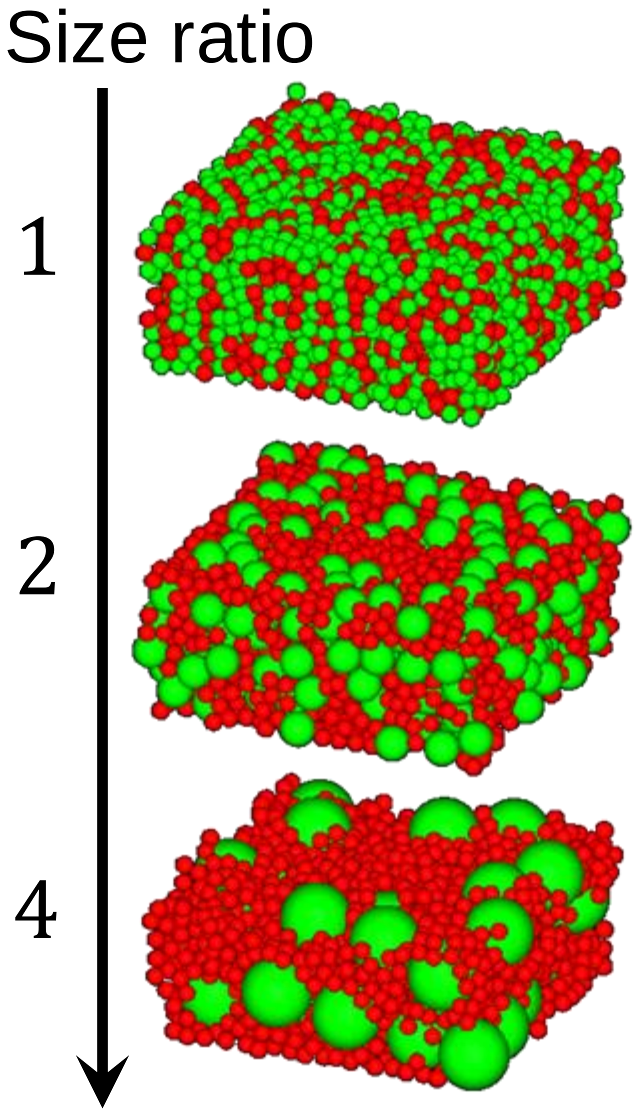
Previous study: Effects of particle size ratio



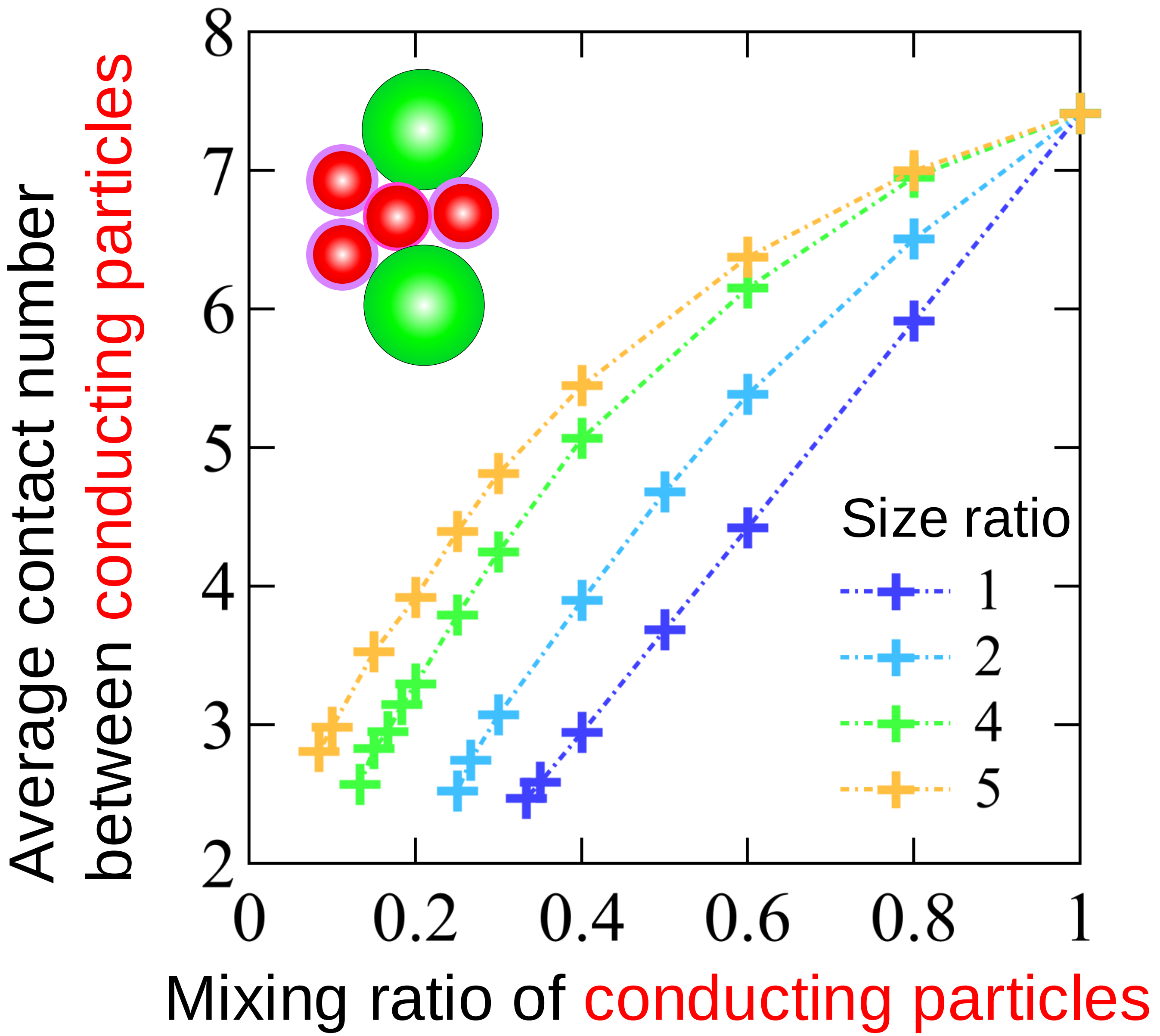
Mixing ratio: 0.4



Previous study: Effects of particle size ratio

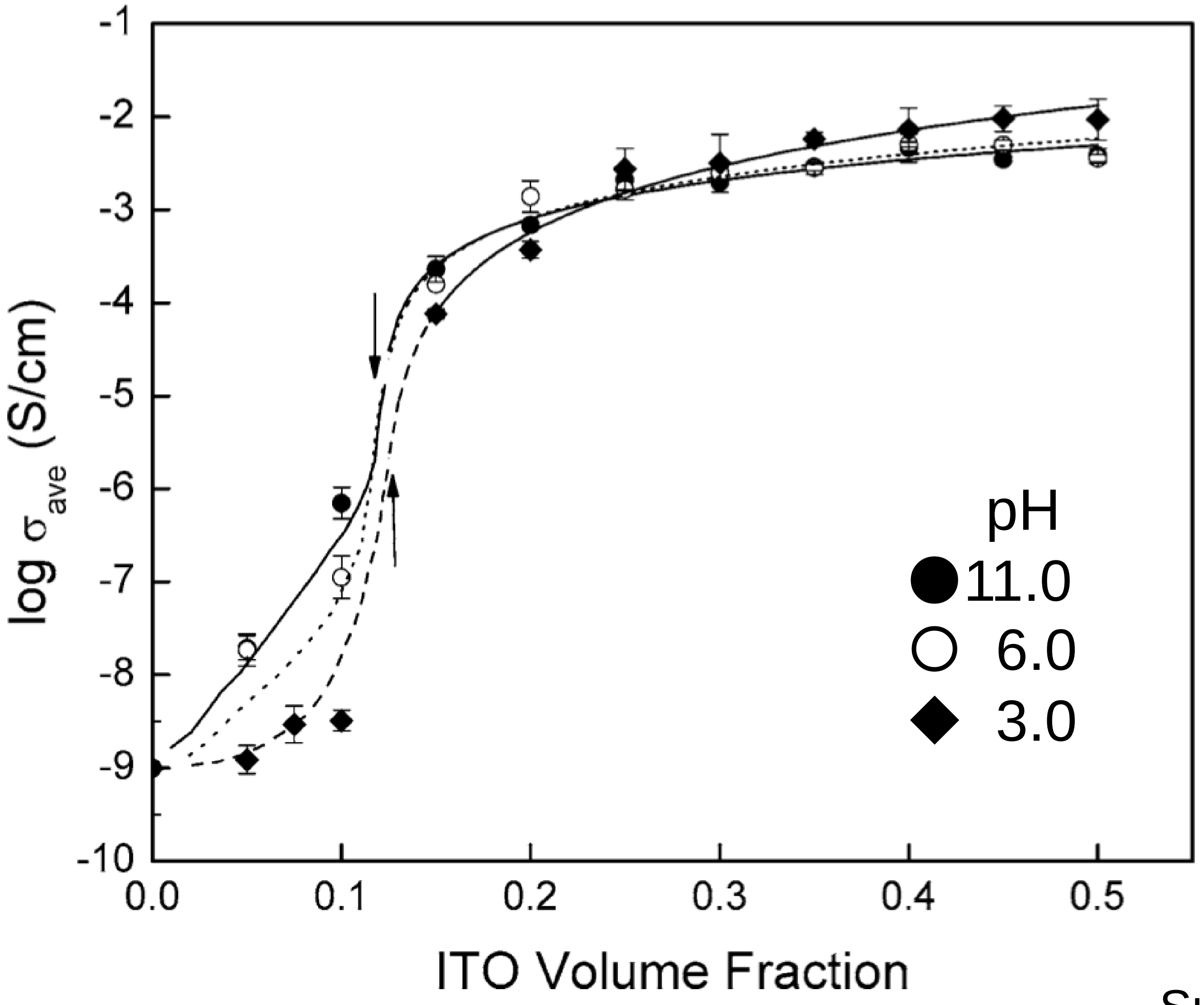


Mixing ratio: 0.4

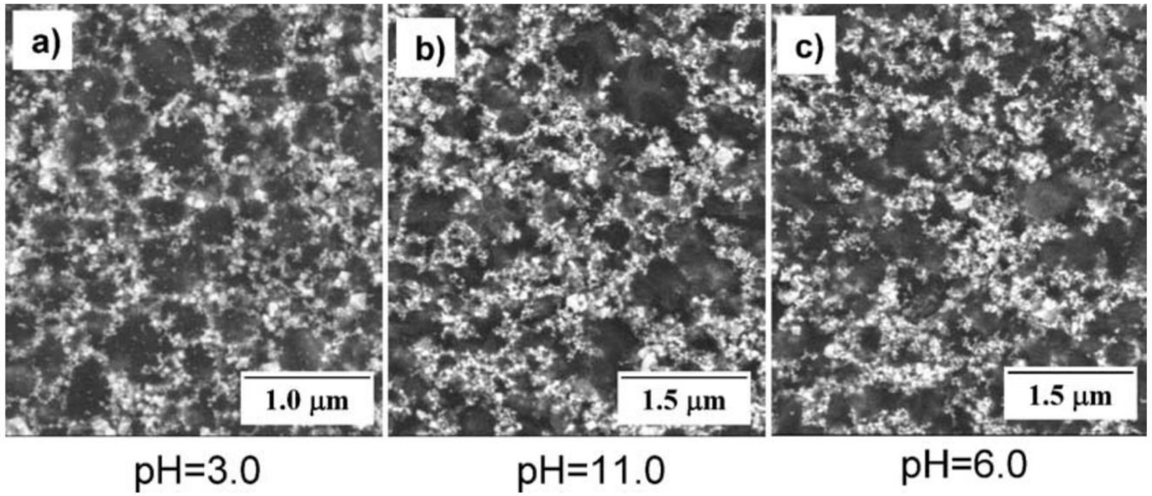


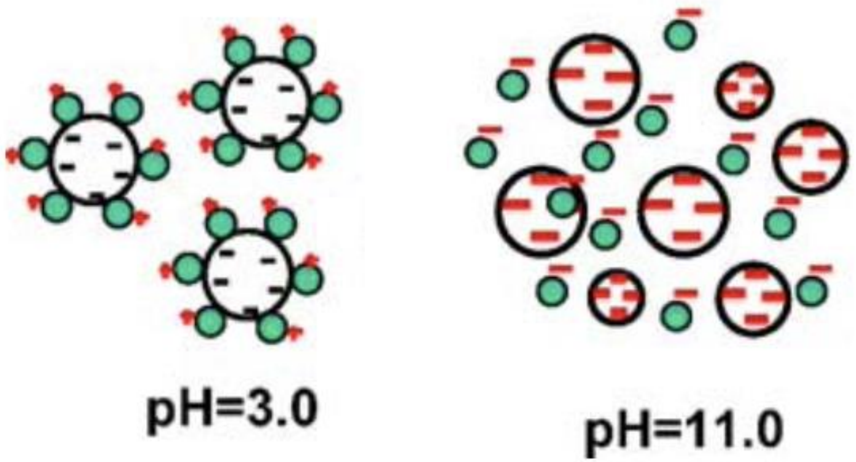
Previous study: Effects of interactions

Aqueous latex/ITO suspensions → Composite coatings



SEM image





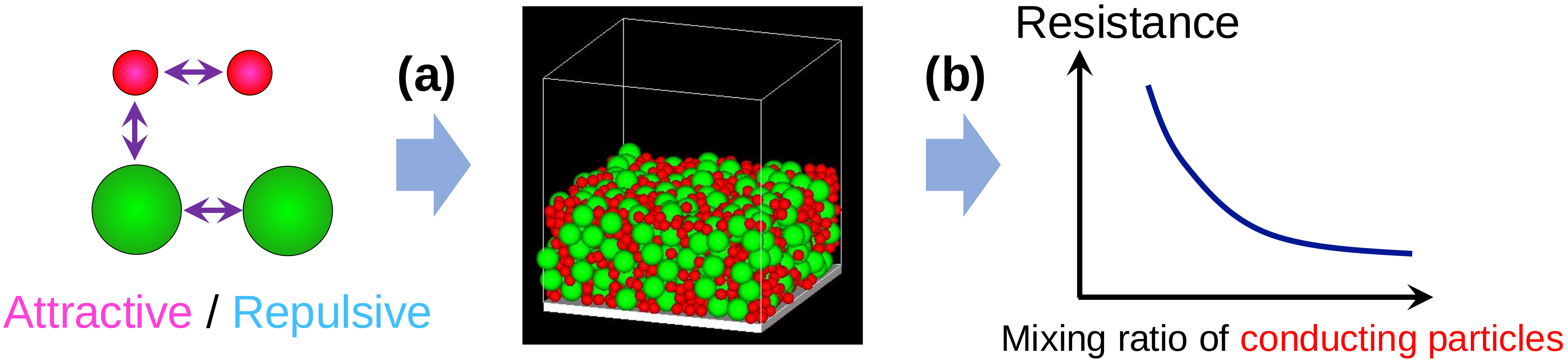
Sun *et al*., J. Colloid Interface Sci. **280**, 387 (2004).

Objective & Method

Investigating the effects of interactions on the conductivity of colloidal films

(a) Numerical simulation analyzing the structure formation of particles during drying

(b) Equivalent circuit modeling to evaluate conductivity



Interactions　　Structure after drying　　Conductivity

Model: Particles' motion

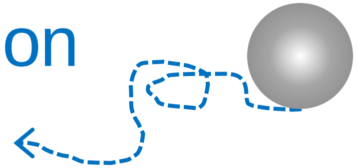
$$m_i \dot{\boldsymbol{v}}_i = -\zeta_i \boldsymbol{v}_i + \boldsymbol{F}_i^{\mathrm{R}} + \boldsymbol{F}_i^{\mathrm{cpl}} + \boldsymbol{F}_i^{\mathrm{cnt}} + \boldsymbol{F}_i^{\mathrm{DLVO}}$$

Fluid Free surface Particles

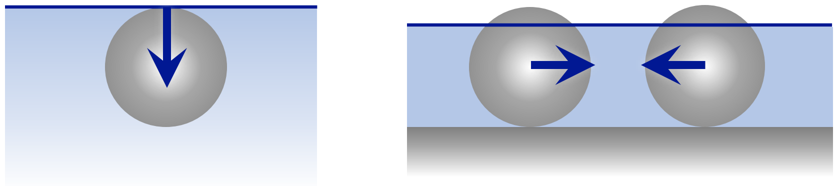
- **Hydrodynamic force**

  Drag: $-\zeta_i \boldsymbol{v}_i$, Fluctuations: $\boldsymbol{F}_i^{\mathrm{R}}$

  → Brownian motion

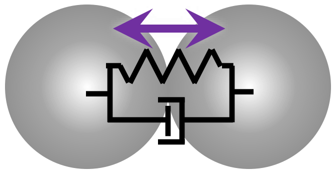


- **Capillary force**: $\boldsymbol{F}^{\mathrm{cpl}}$

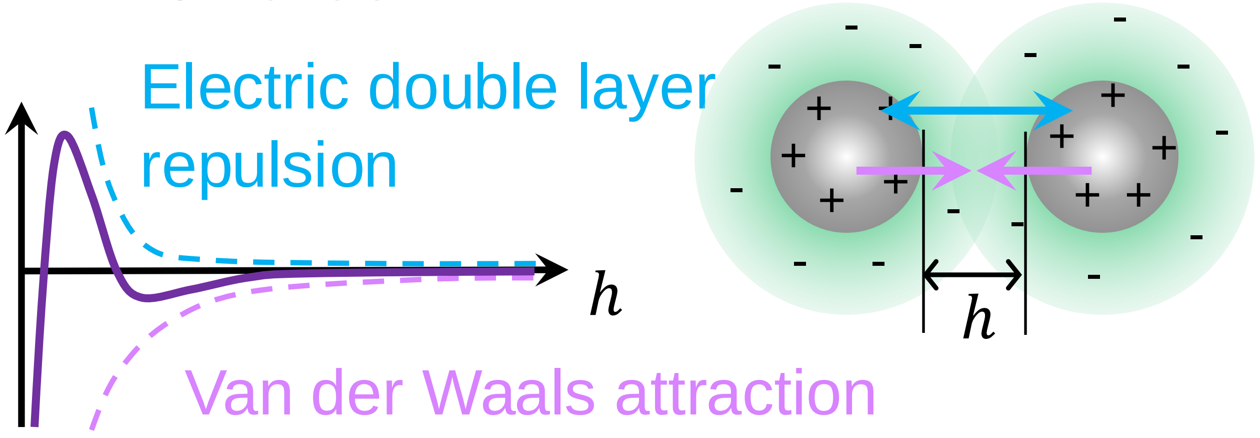


Vertical Lateral

- **Contact force**: $\boldsymbol{F}^{\mathrm{cnt}}$



- **DLVO force**: $\boldsymbol{F}^{\mathrm{DLVO}}$



Evaluation of conductivity

Kirchhoff's current law

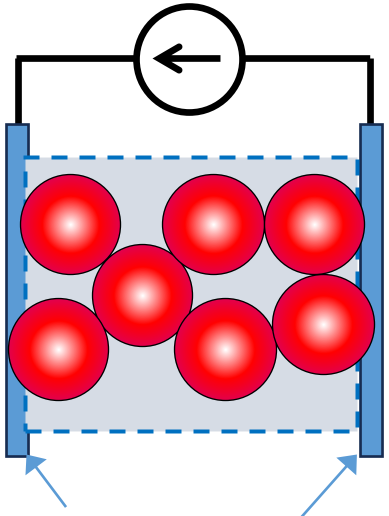
$$\sum_j \frac{V_i - V_j}{R_{ij}} = I\delta_{i0}$$

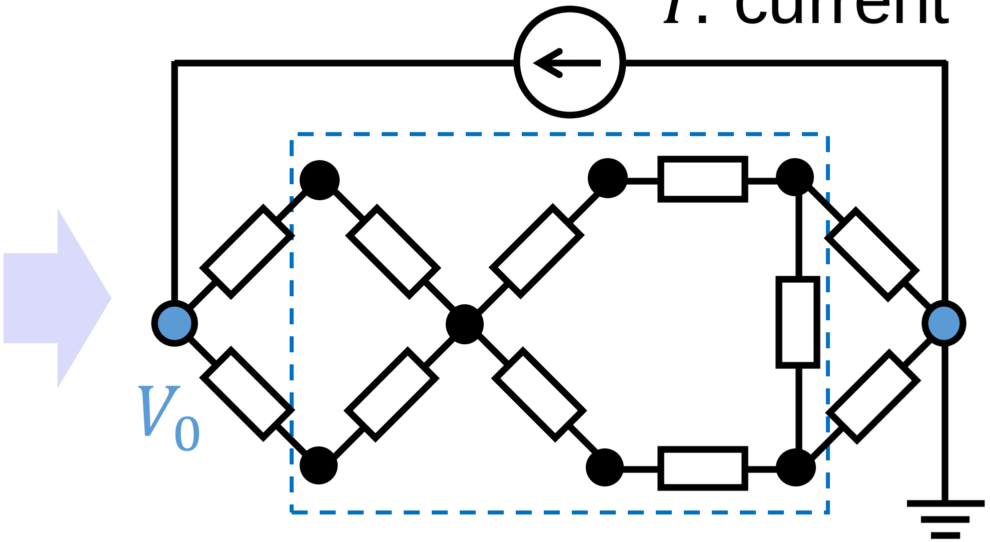
$$(i = 0, 1, \dots, N+1)$$

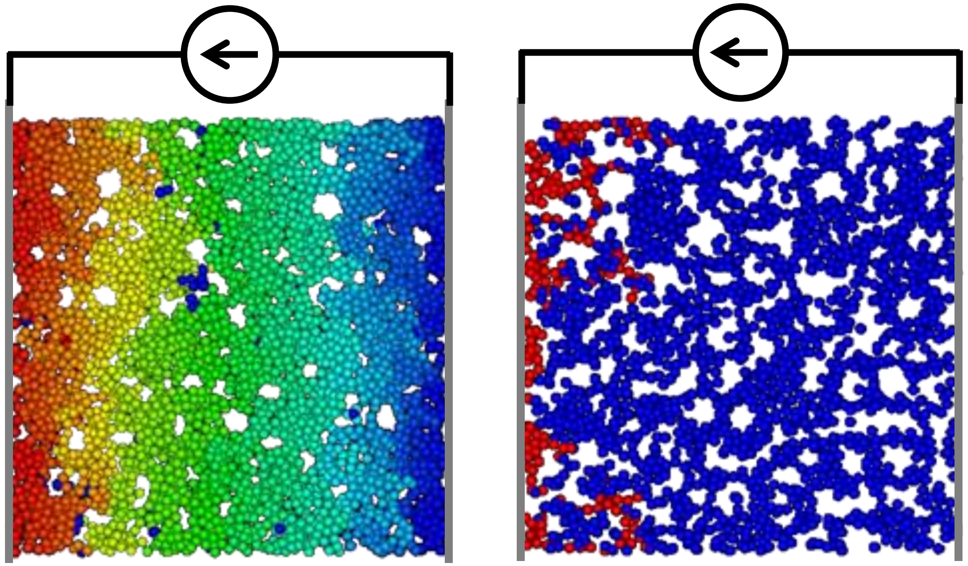
Resistance between nodes

$$R_{ij} = \begin{cases} r & \text{connected} \\ \infty & \text{disconnected} \end{cases}$$

→ Sheet resistance $R = \dfrac{V_0}{I}$





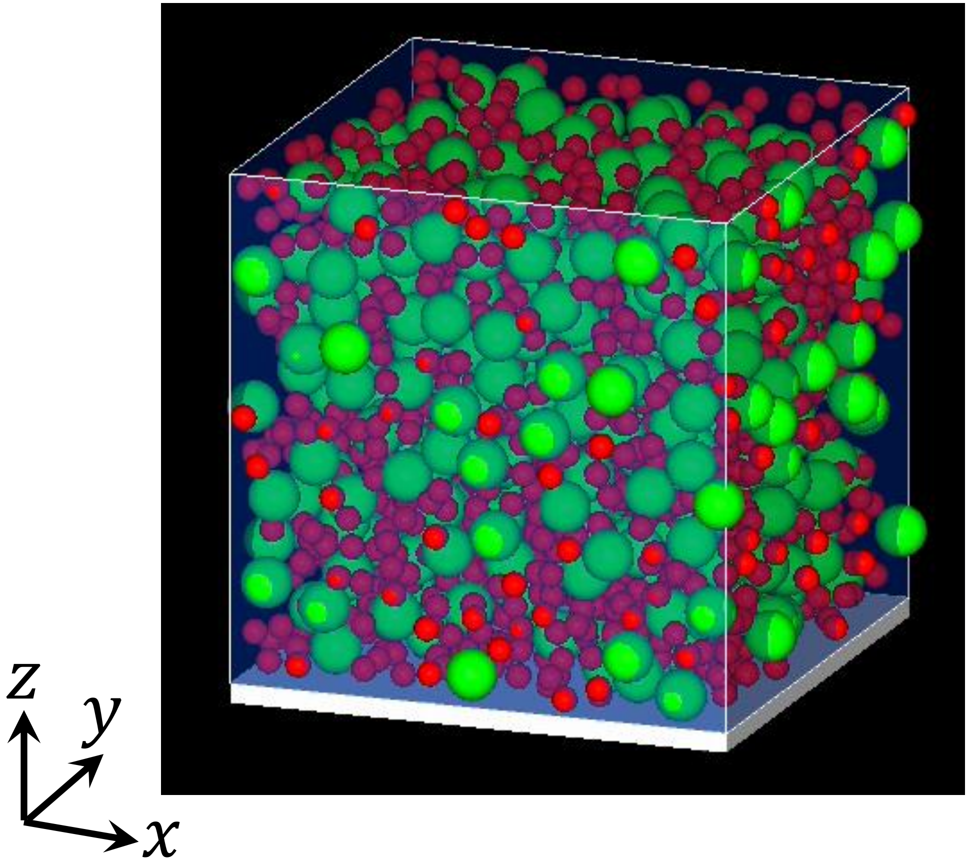


No conducting paths → $R = \infty$

Simulation conditions

Conducting / Insulating particles

- Diameter: **C**: $d = 20\ \mathrm{nm}$, **I**: $2d = 40\ \mathrm{nm}$
- Initial volume fraction: $\phi_\mathrm{C} + \phi_\mathrm{I} = 0.3$
- Mixing ratio: $\alpha_\mathrm{C} = \frac{\phi_\mathrm{C}}{\phi_\mathrm{C}+\phi_\mathrm{I}} = 0.1 - 1$
- Zeta potential: three conditions



System size: $20d \times 20d \times 20d$

Fluid: water

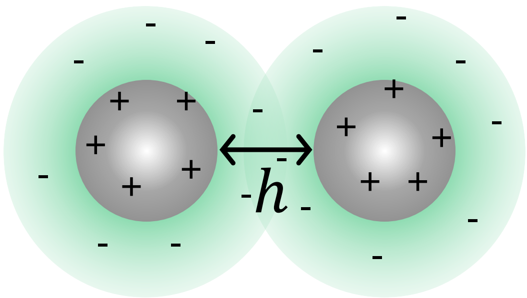
- Particle drying Péclet number (**C**)

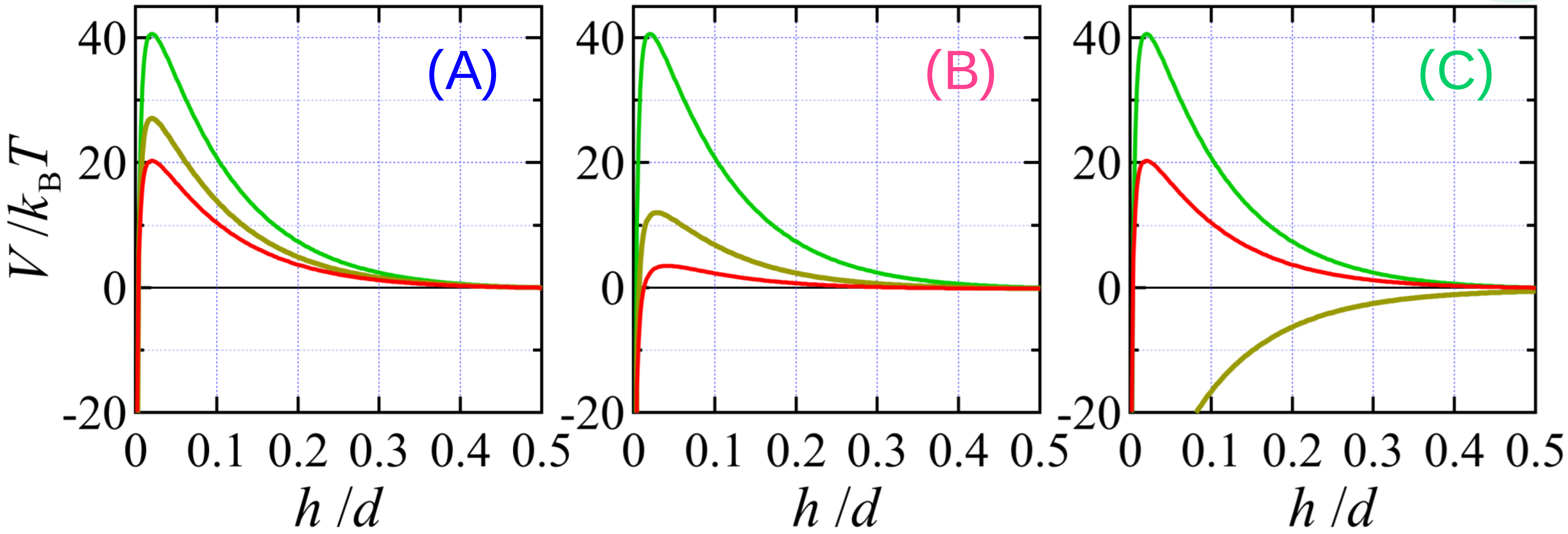
$$\mathrm{Pe} = \frac{(\text{Drying rate})}{(\text{Diffusion rate})} = \frac{U}{D/d} = 10$$

Simulation conditions: DLVO potentials

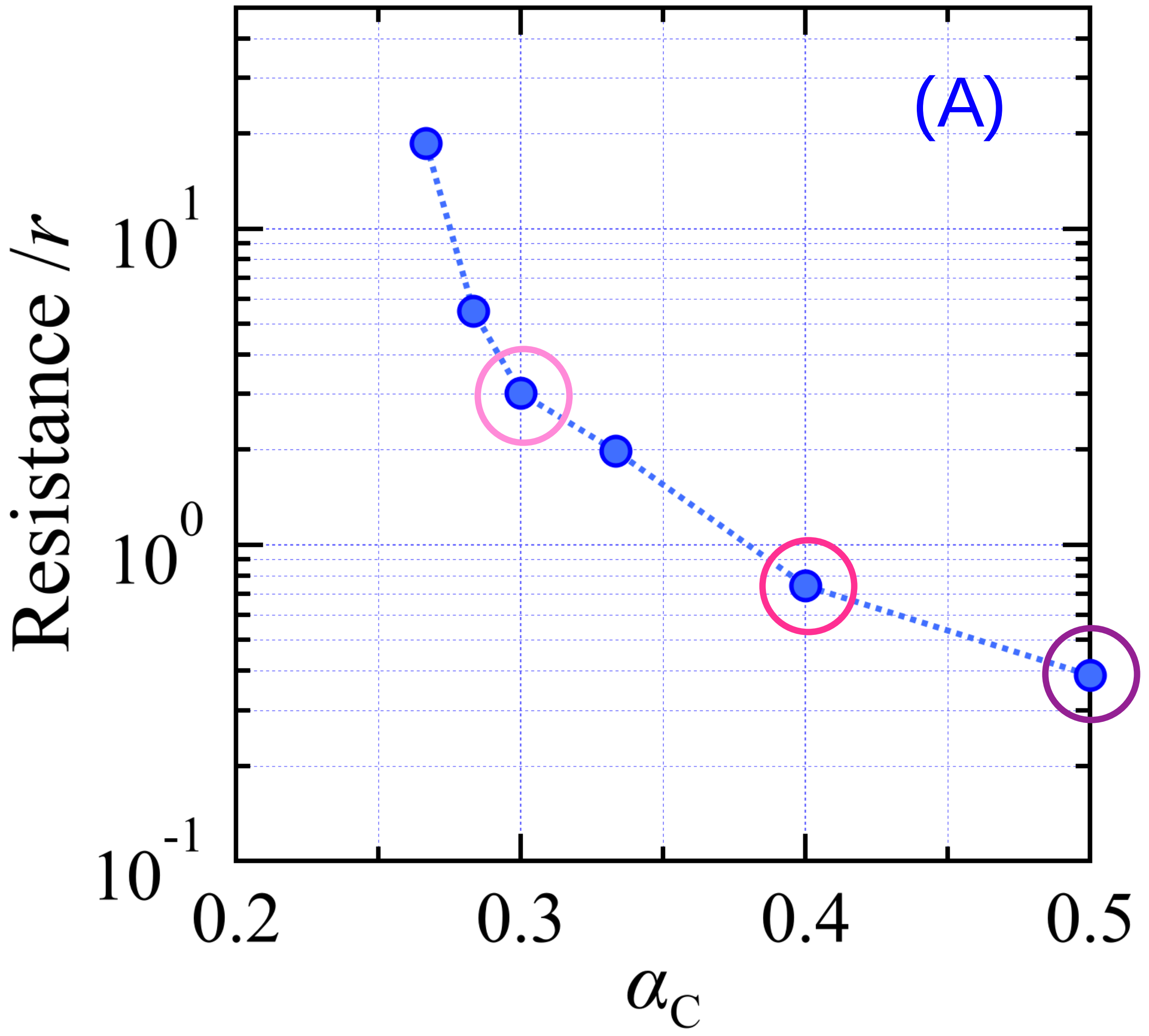
Condition	Zeta potential /mV		Interaction		
	C	**I**	**C-C**	**I-I**	**C-I**
A	60	60	R	R	R
B	30	60	A	R	R
C	60	-60	R	R	A

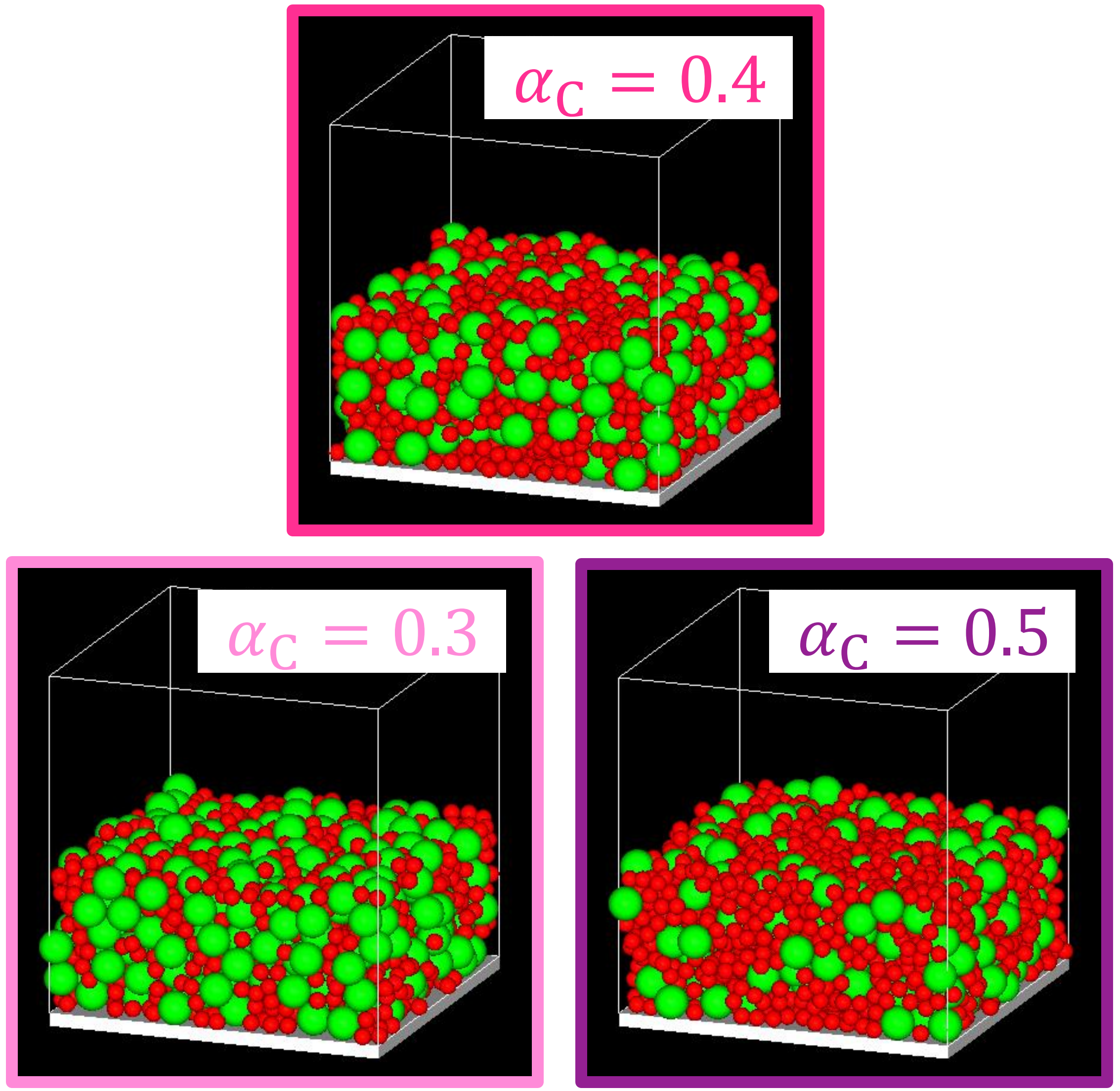
Attractive
Repulsive



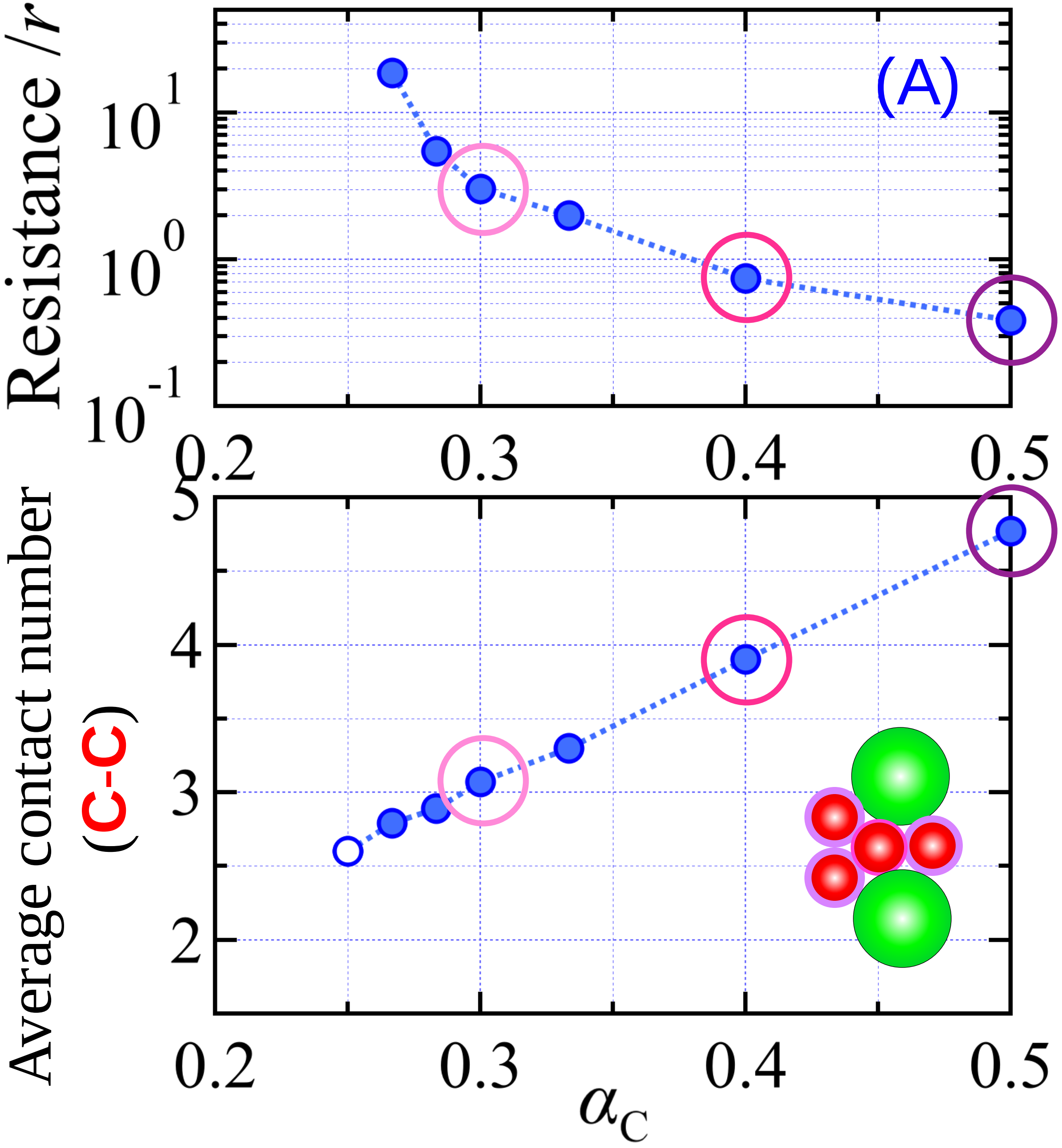


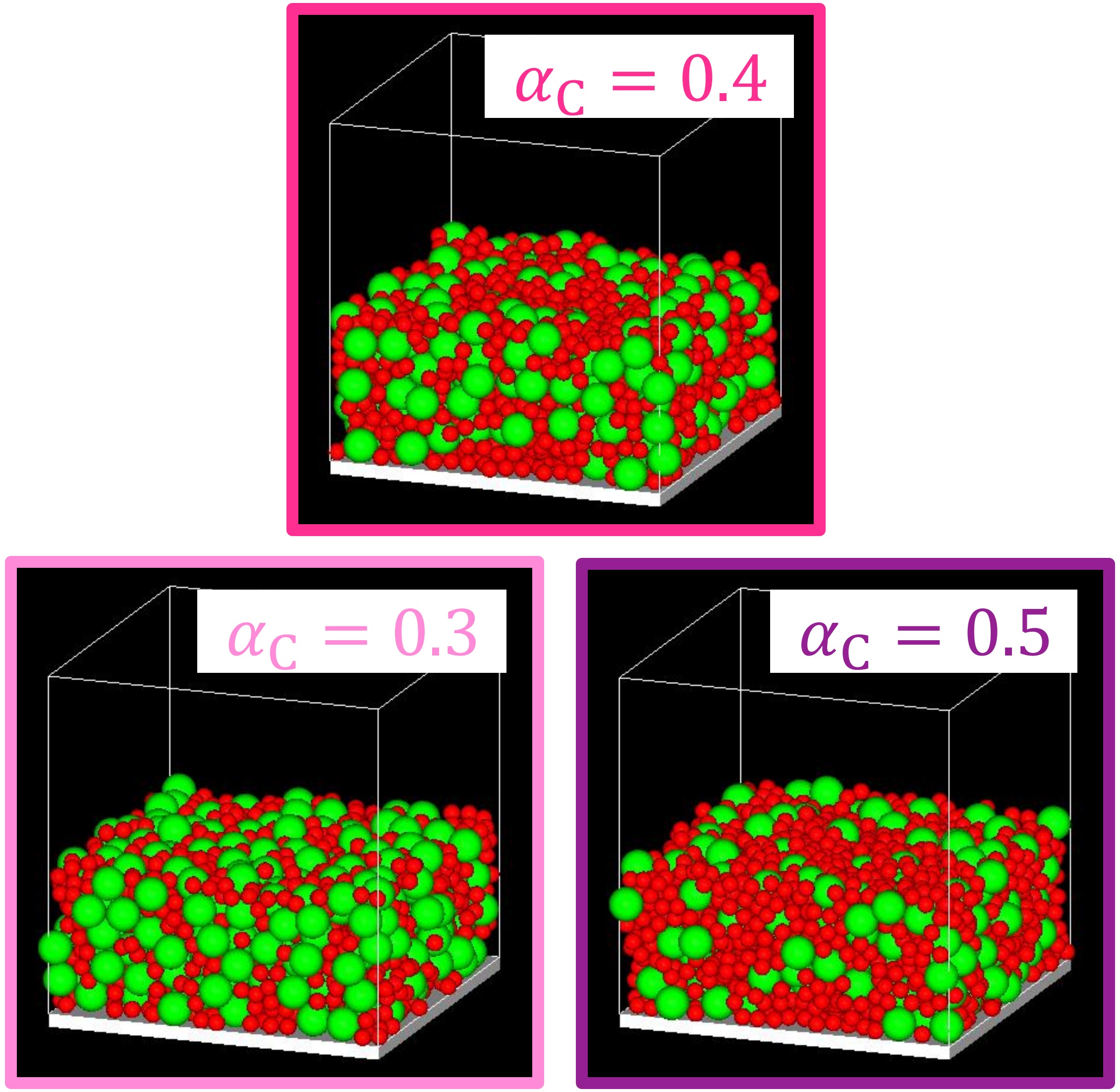
Conductivity



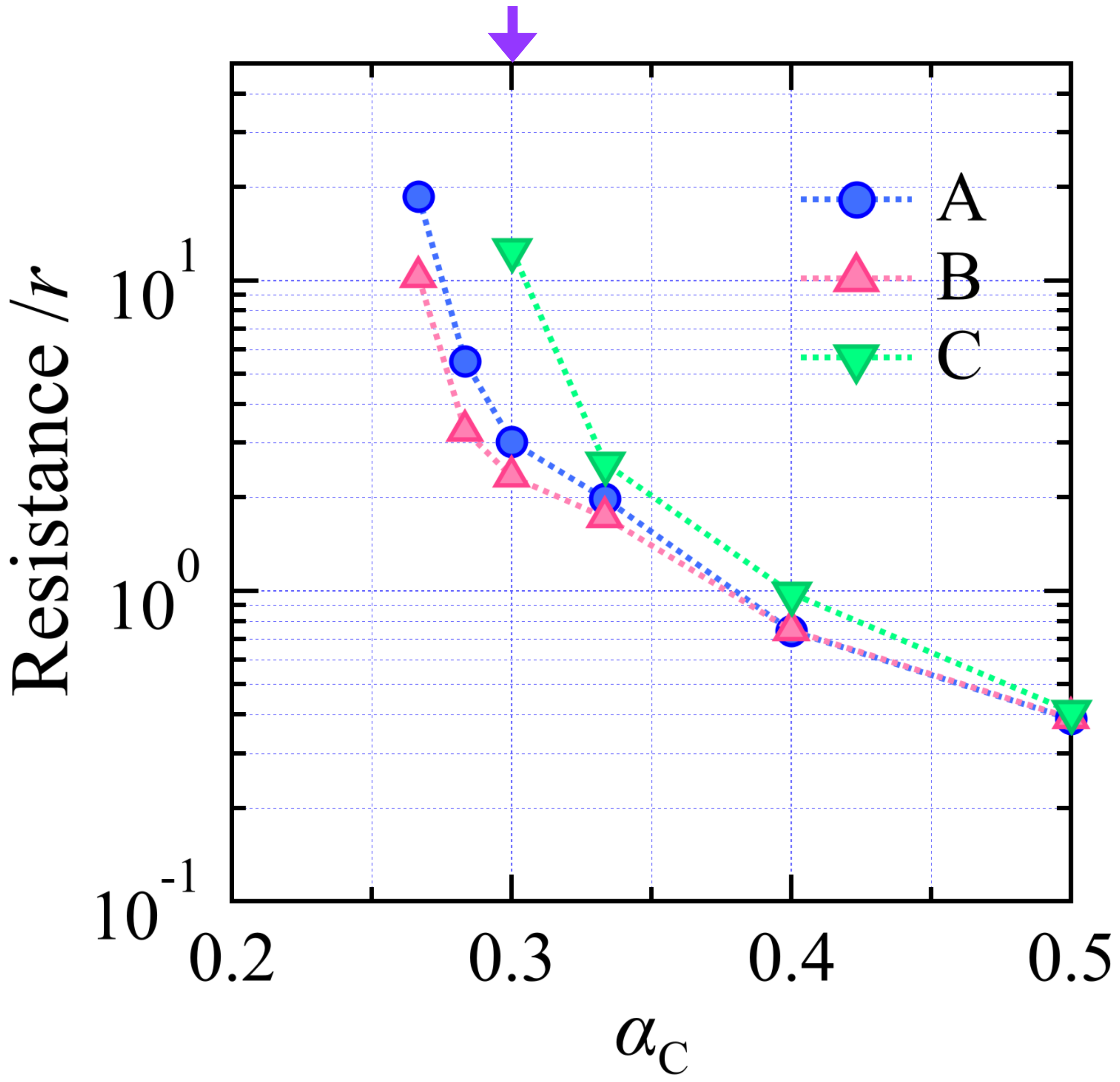


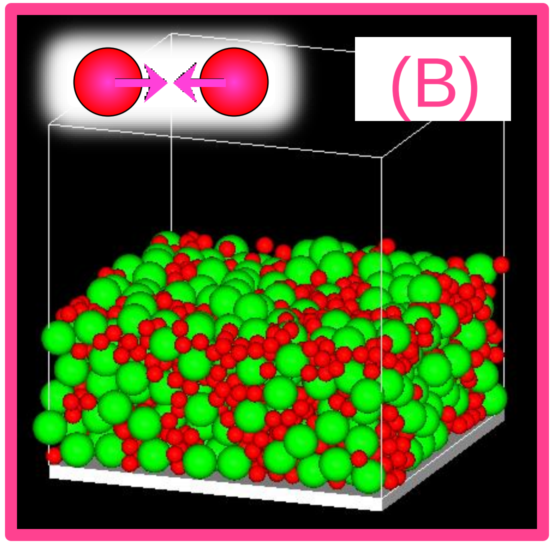
Contact number (C-C)

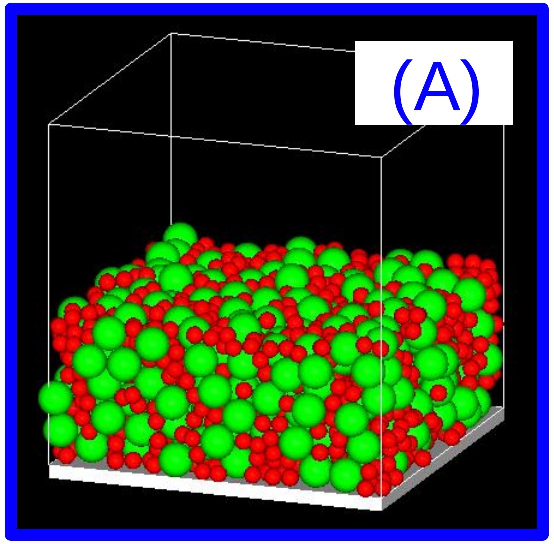


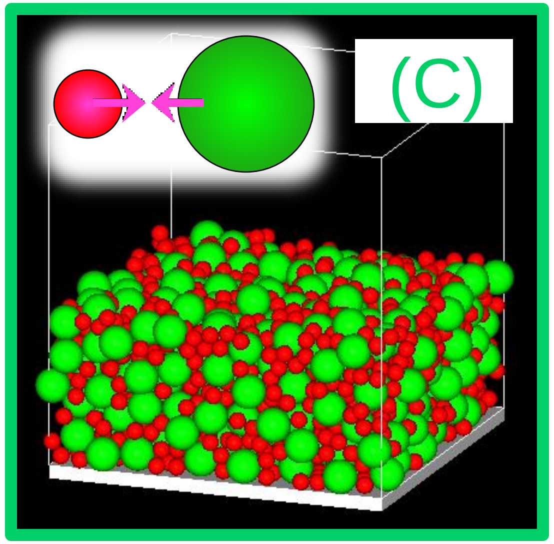


Conductivity









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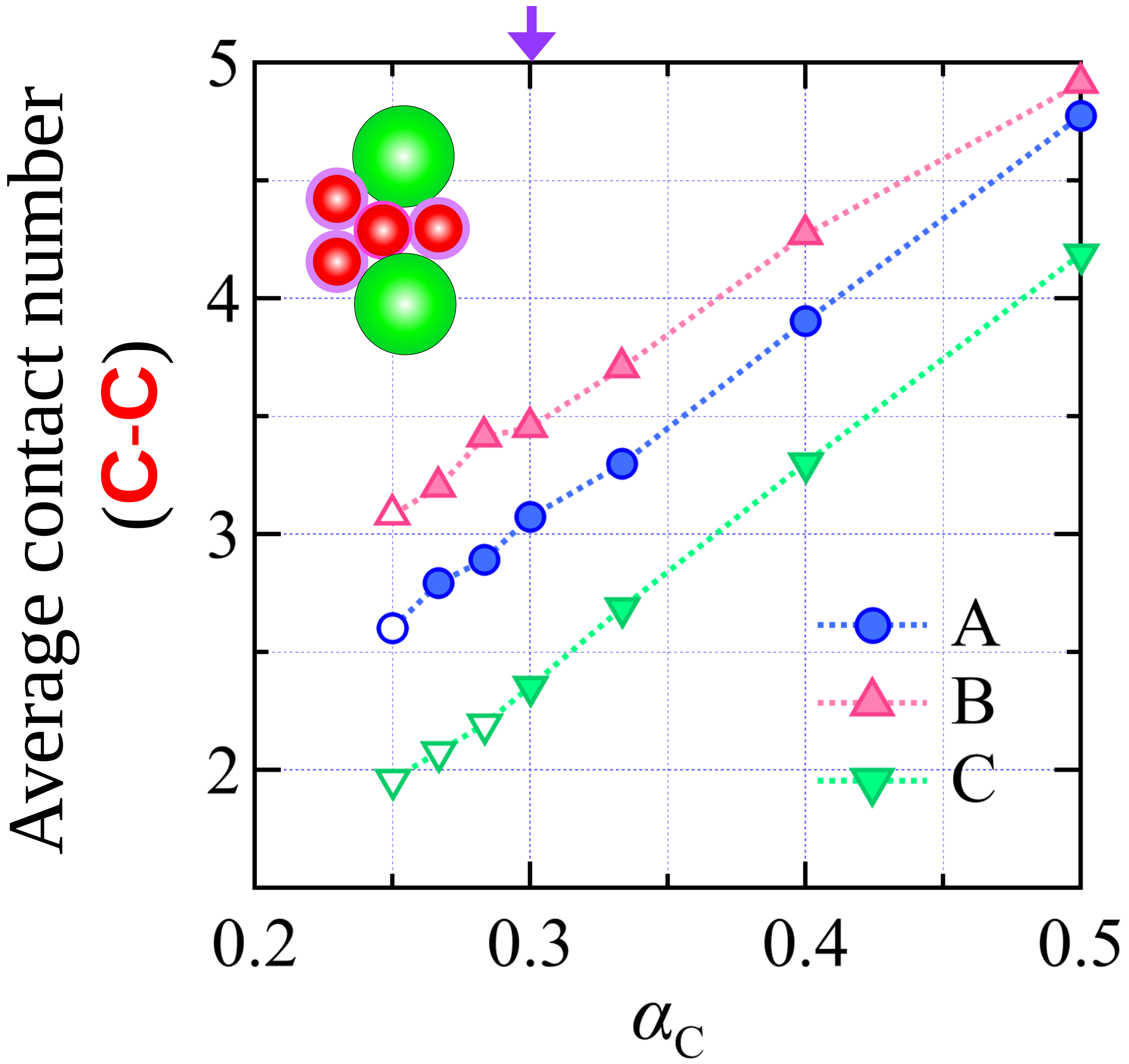
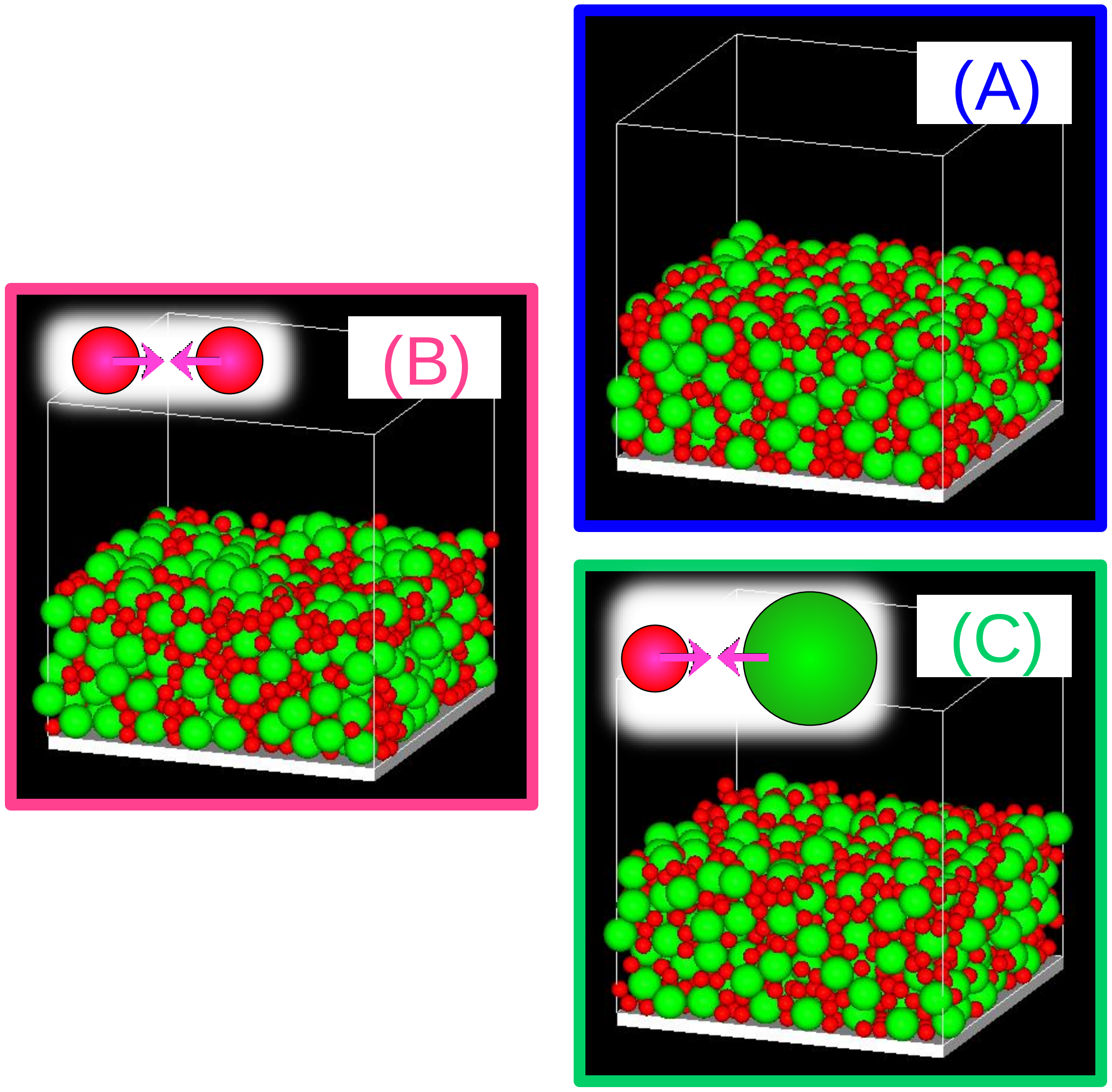
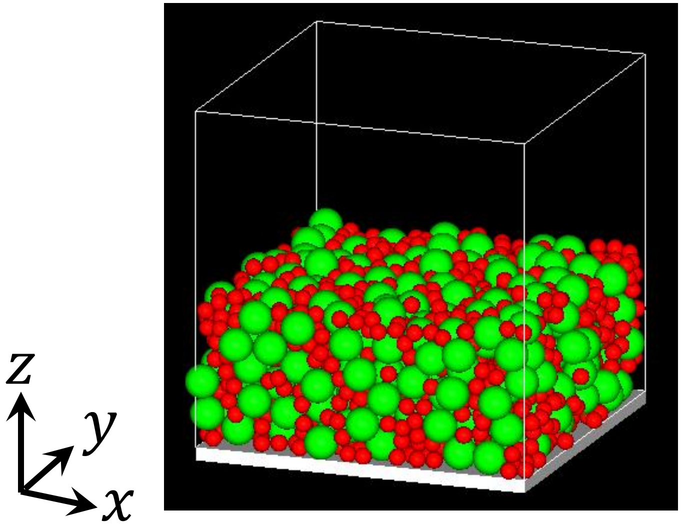
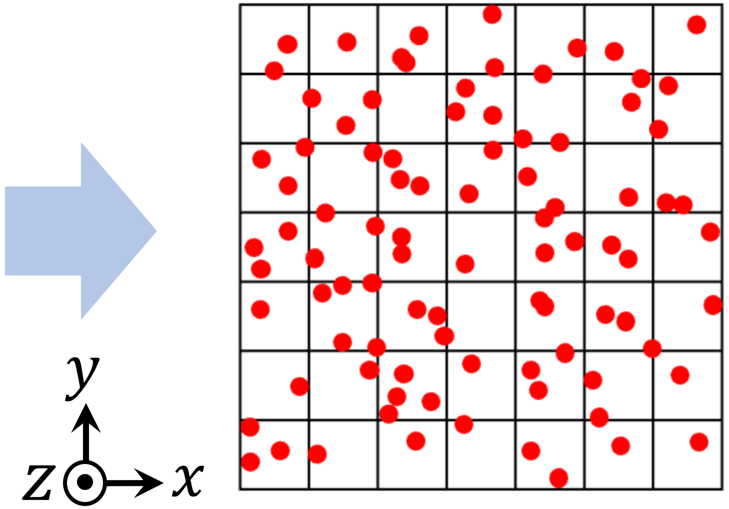




Morisita's index: I_δ



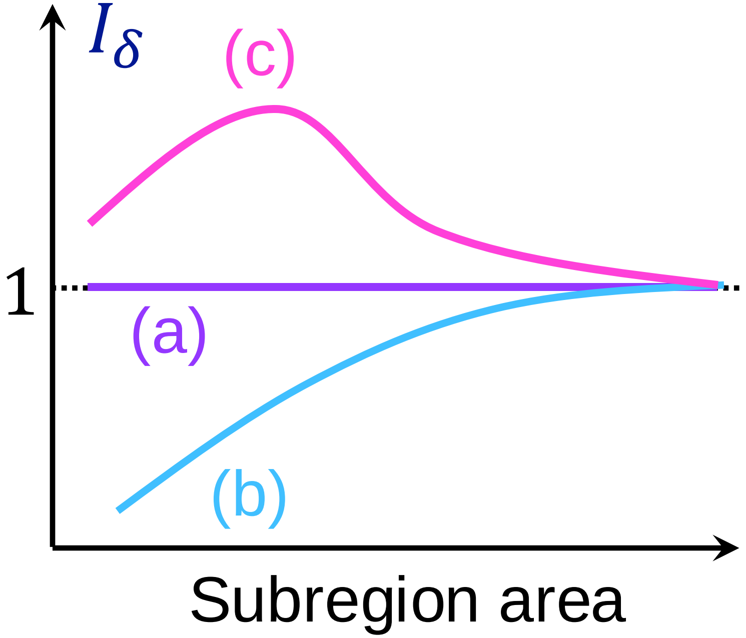


Projection onto xy plane

Division into q subregions

$$I_\delta = q \frac{\sum_{j=1}^{q} n_j (n_j - 1)}{N(N-1)}$$

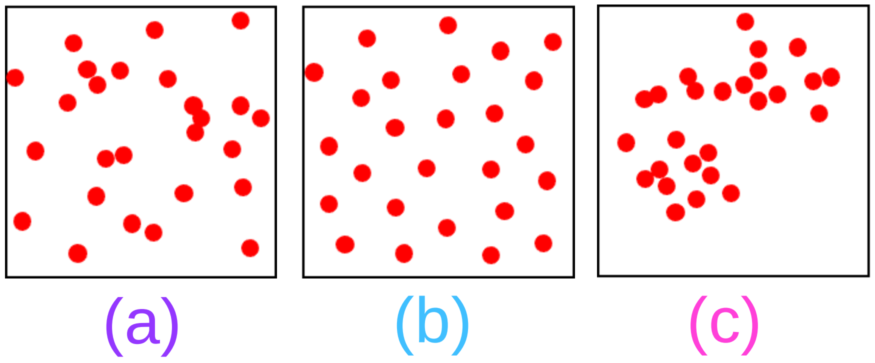
n_j : number of particles in j-th subregion



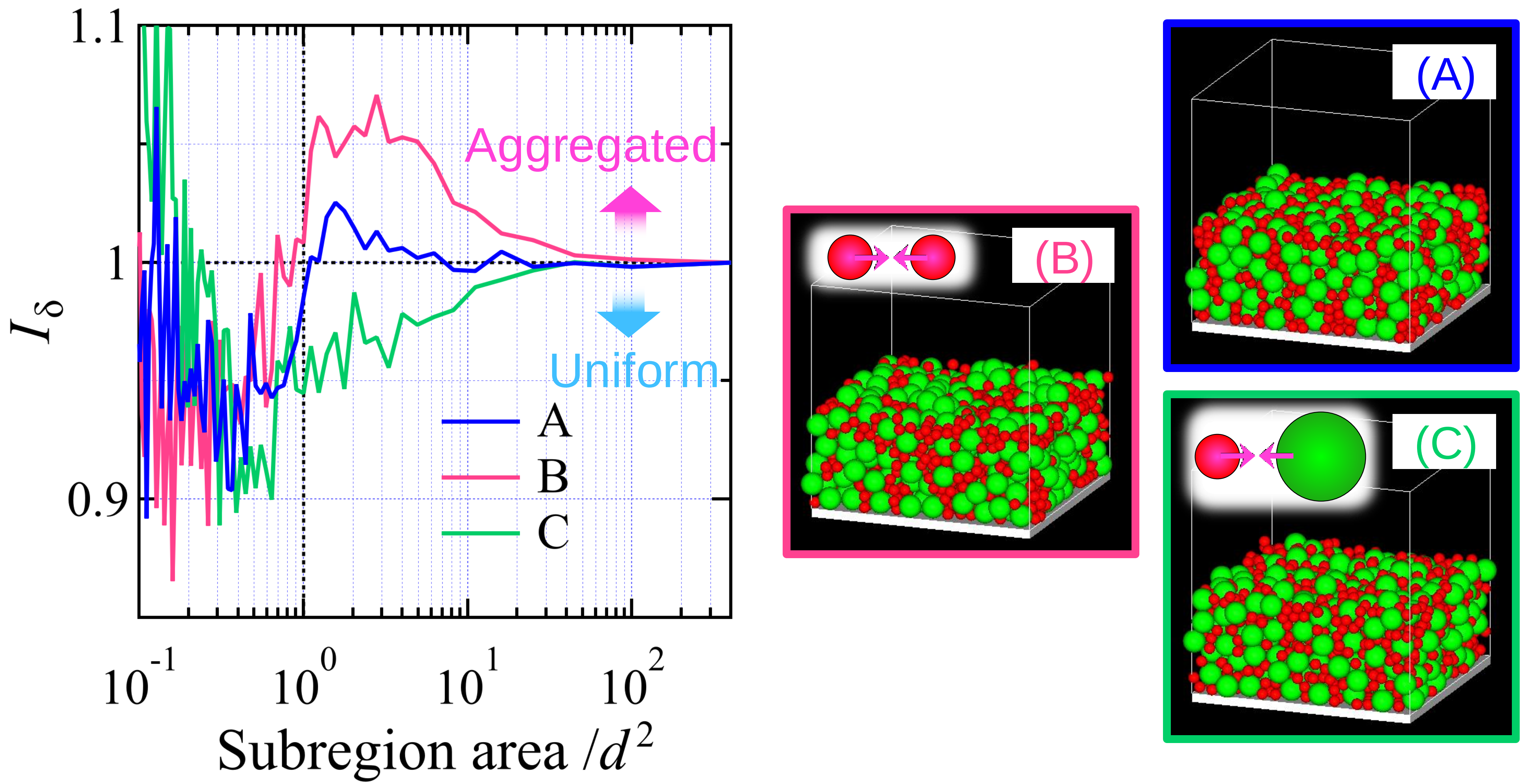
(a) Random → $I_\delta = 1$

(b) Uniform → $I_\delta < 1$

(c) Aggregated → $I_\delta > 1$



Distribution of particles (C)

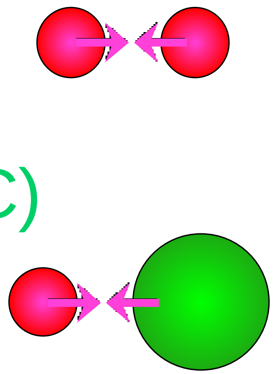


Summary

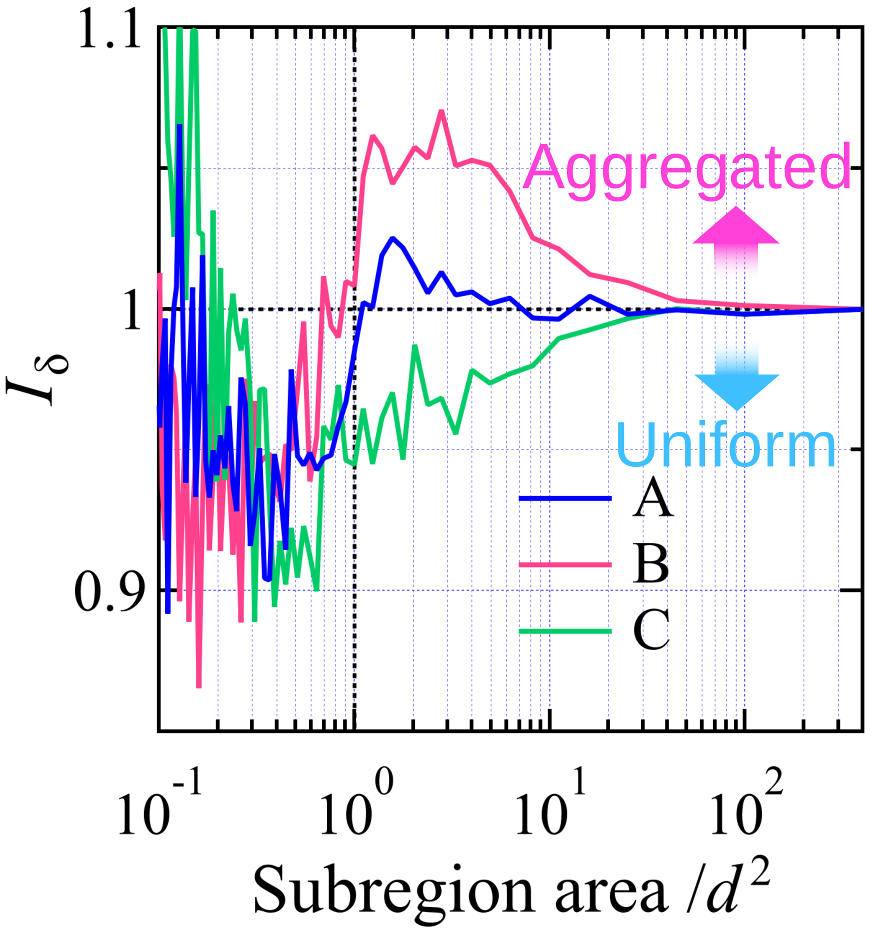
(A) No

(B)

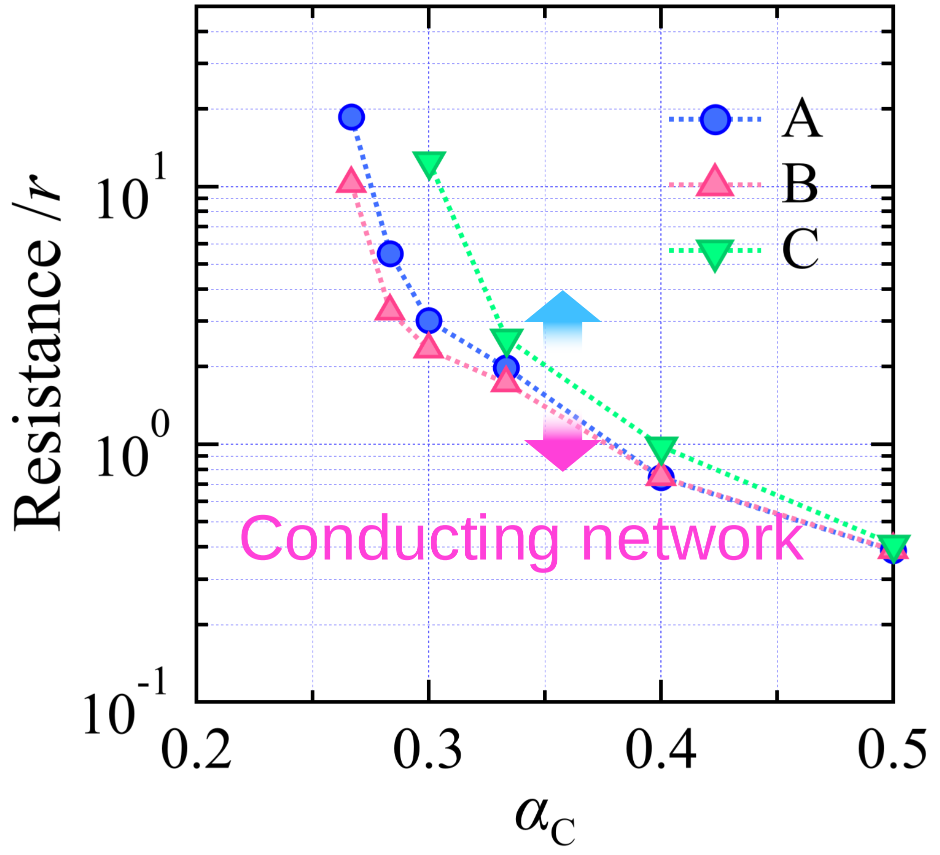
(C)



Attractive interactions



Distribution of conducting particles



Conductivity (Resistance)