Paintistanbul & Turkcoat Congress
05-06 December 2023

KANSAI PAINT

Development of conductive assistant slurry for lithium-ion batteries based on coating technologies

Kansai Paint Co.,Ltd.
Corporate Research and Development
Research and Development Division

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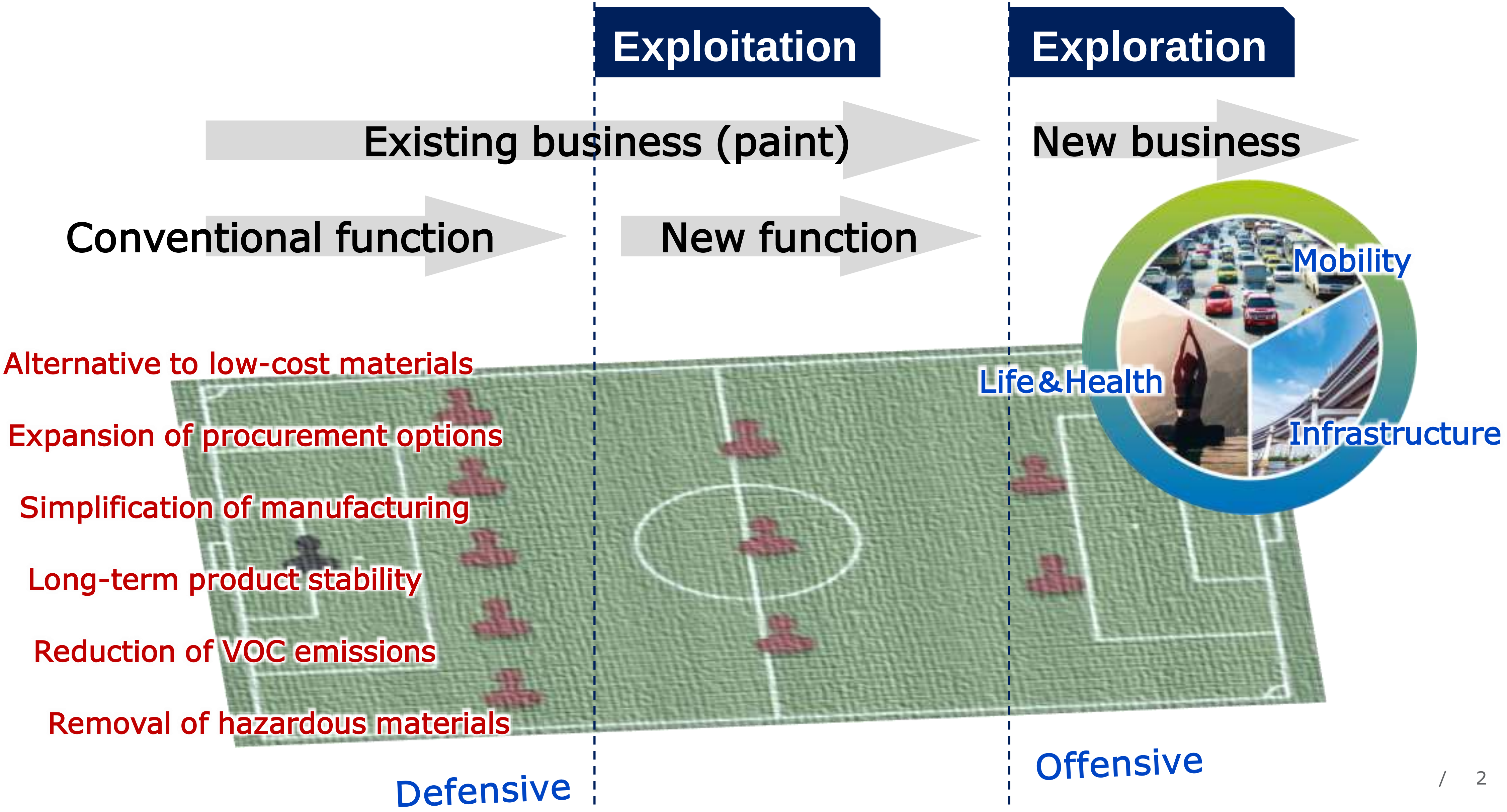
Ambidexterity strategy in KANSAI paint



Core technologies and challenges of new business

Core technologies

- Polymer structure control
- Photosensitive film or material
- Surface functionalization
- Lamination control
- Polymer design
- Emulsion polymerization
- Rheology control
- Coating process design
- Multilayer film forming
- Formulation design
- Particle dispersing
- Adhesion or exfoliation
- Drying process design
- Anti-corrosion
- Total coordination of multilayer
- Powder blending
- Pigment selection
- Gas/ion barrier
- Prediction, Computing
- Durability

Potential value propositions

- Antifouling, Easy-clean
- Bio-repellent, Bio-affinity
- Water-repellent, Water-affinity
- Anti-icing
- Fire-resistant, Fire-extinguishing
- Heat-resistant, Heat-conduction, Heat-shielding
- Conducting, Insulating, Dissipating
- Slippery, Friction
- Long-term-durability
- Functional-slurry

Exploration of potential market or new business frontier

Potential entry opportunities in LIB industry

TOYOTA Yaris HV

Customer

CAGR=roughly 15-20% through 2030
according to Market researchers' estimates

- Rapid market growth
- Insatiable technological evolution
- Various functional coating possibilities

Company

e.g. Pigment dispersion or
Coating workability improvement

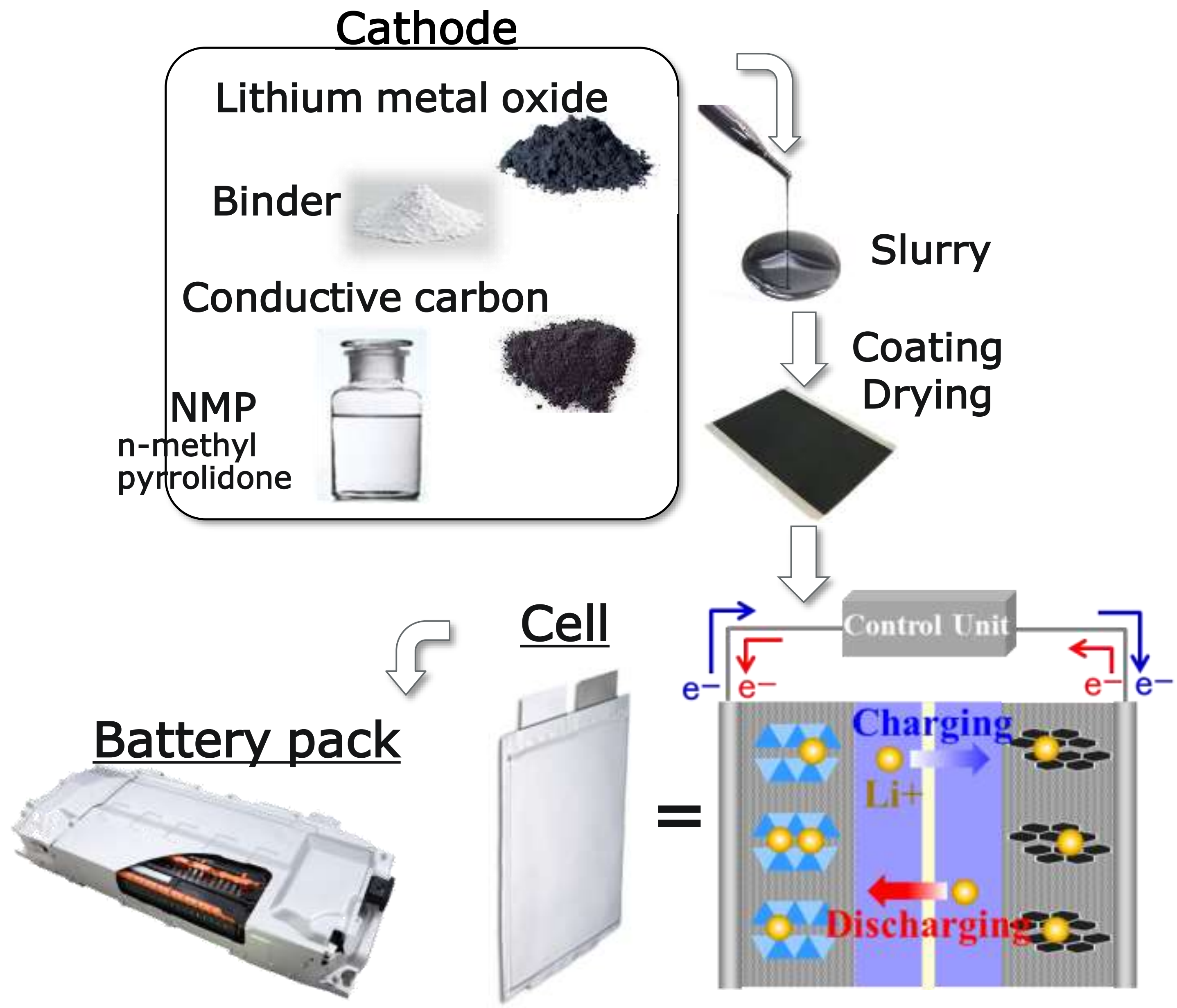
- Affinity with core technologies of paint industry
- Sales channels to automobile/parts manufacturers

Competitor

e.g. Inks, Adhesives field

- Approaches from other industries with similar technologies
- In-house development by battery manufacturers

LIB cathode manufacturing process



Cathode manufacturing process

KANSAI 's stage

Carbon
Binder
NMP
Dispersant
→ Dispersing → CC paste

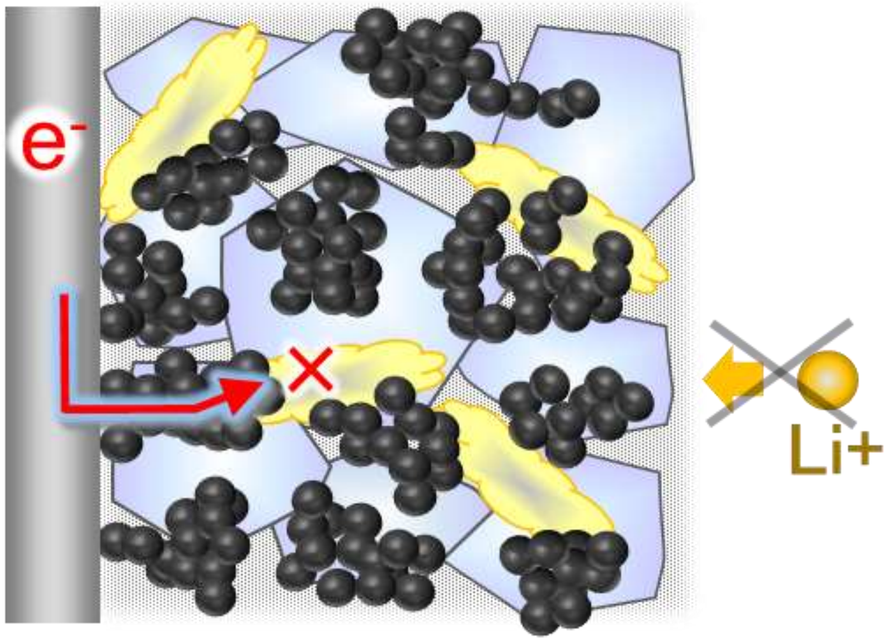
User's stage

Li-metal oxide → Mixing → Cathode Slurry

CC paste：Conductive carbon paste

Ideal dispersing state for conductive carbon black

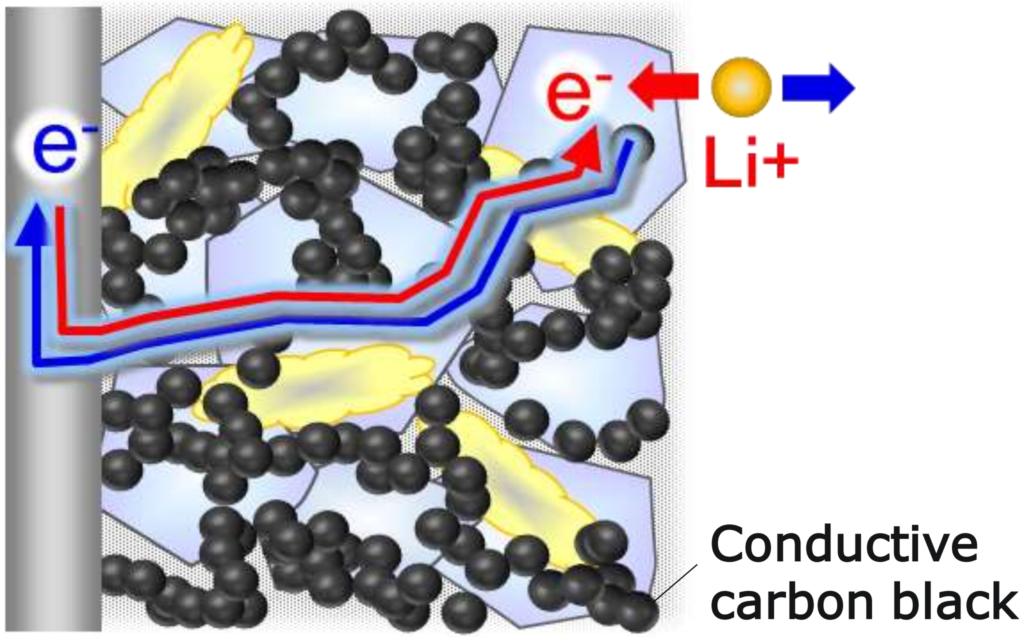
Insufficient dispersing



Carbon aggregated

= hard for electron to move

Ideal dispersing



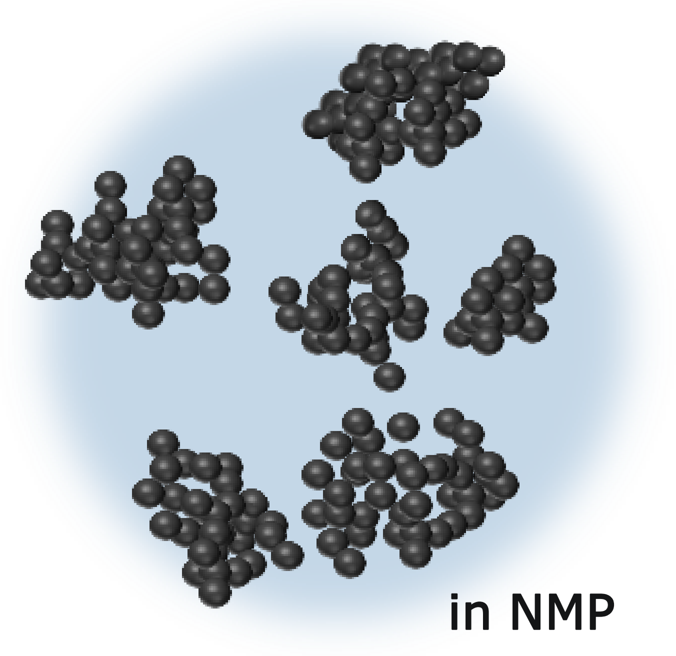
Carbon chained

= easy for electron to move

Problems of CC paste with insufficient dispersing

CC paste：Conductive carbon paste

Insufficient dispersing

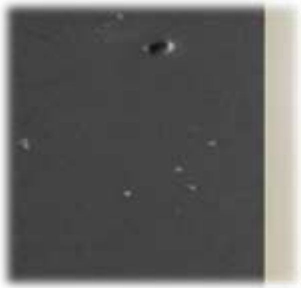


1. Carbon caking in CC paste
2. Thickening of CC paste
3. Filtration trouble of CC paste
4. Defects on cathode film
5. Poor battery performance

Caking

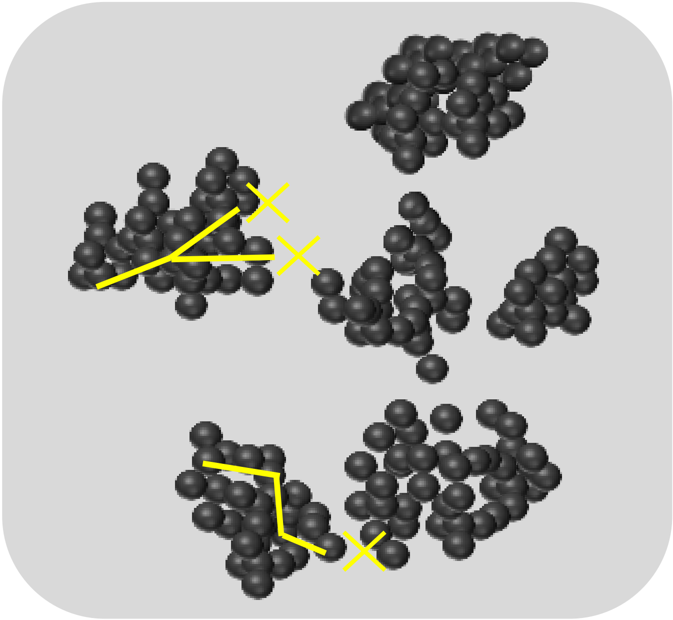
Thickening

Film defect (e.g. hole)

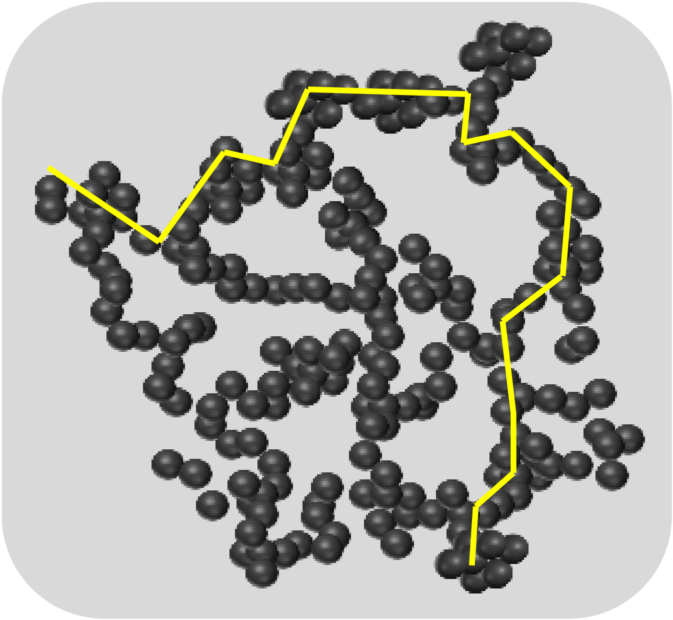


Importance of dispersion control for carbon

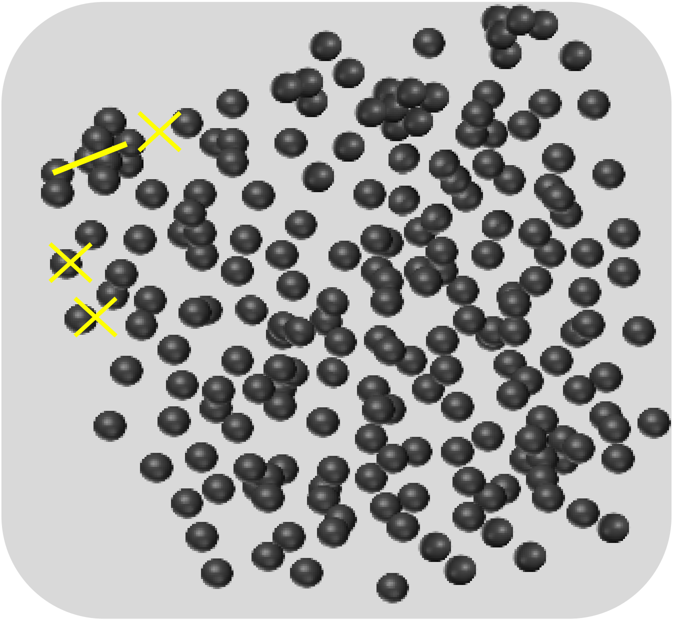
Insufficient dispersing



Ideal dispersing



Excess dispersing



Good battery performance

Development of suitable conductive carbon paste

- Design of high-performance dispersants
- Optimization dispersing process

Affinity of functional groups for graphite

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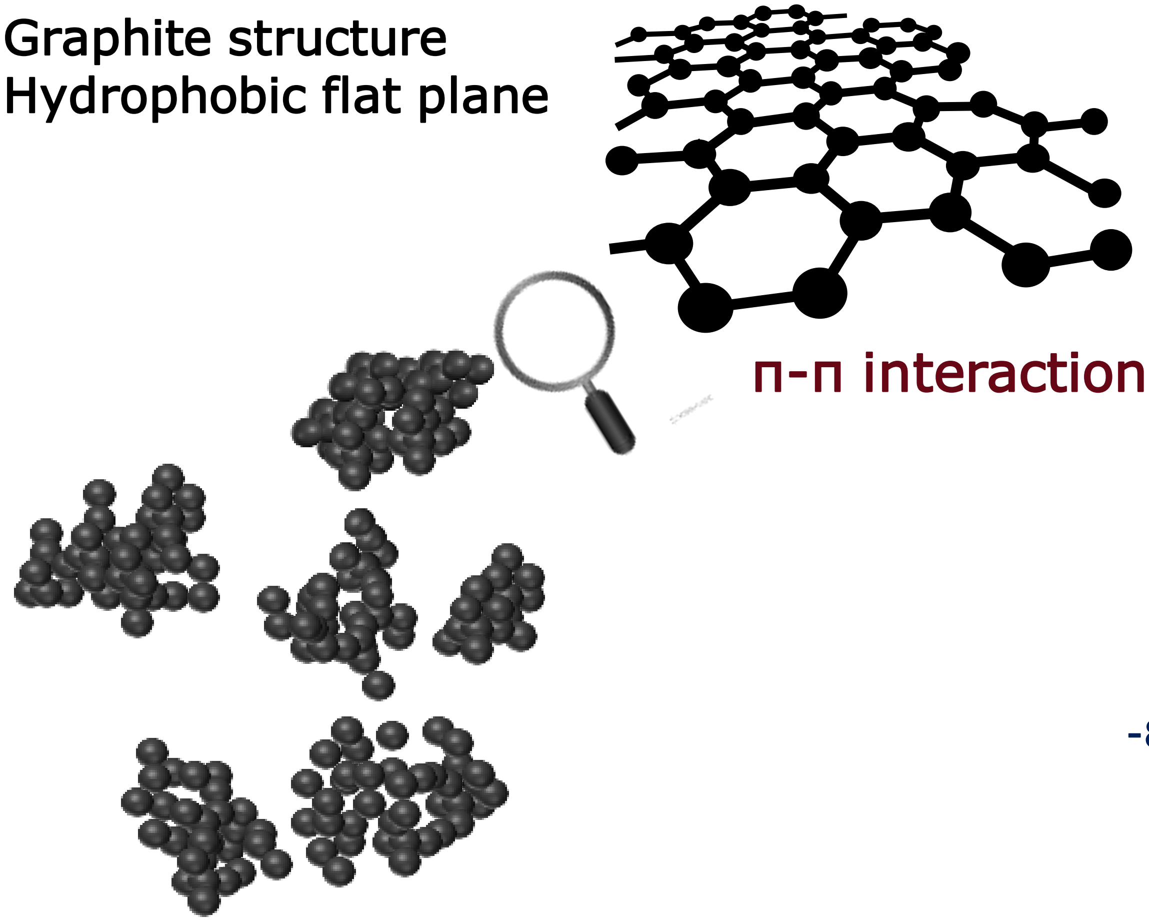
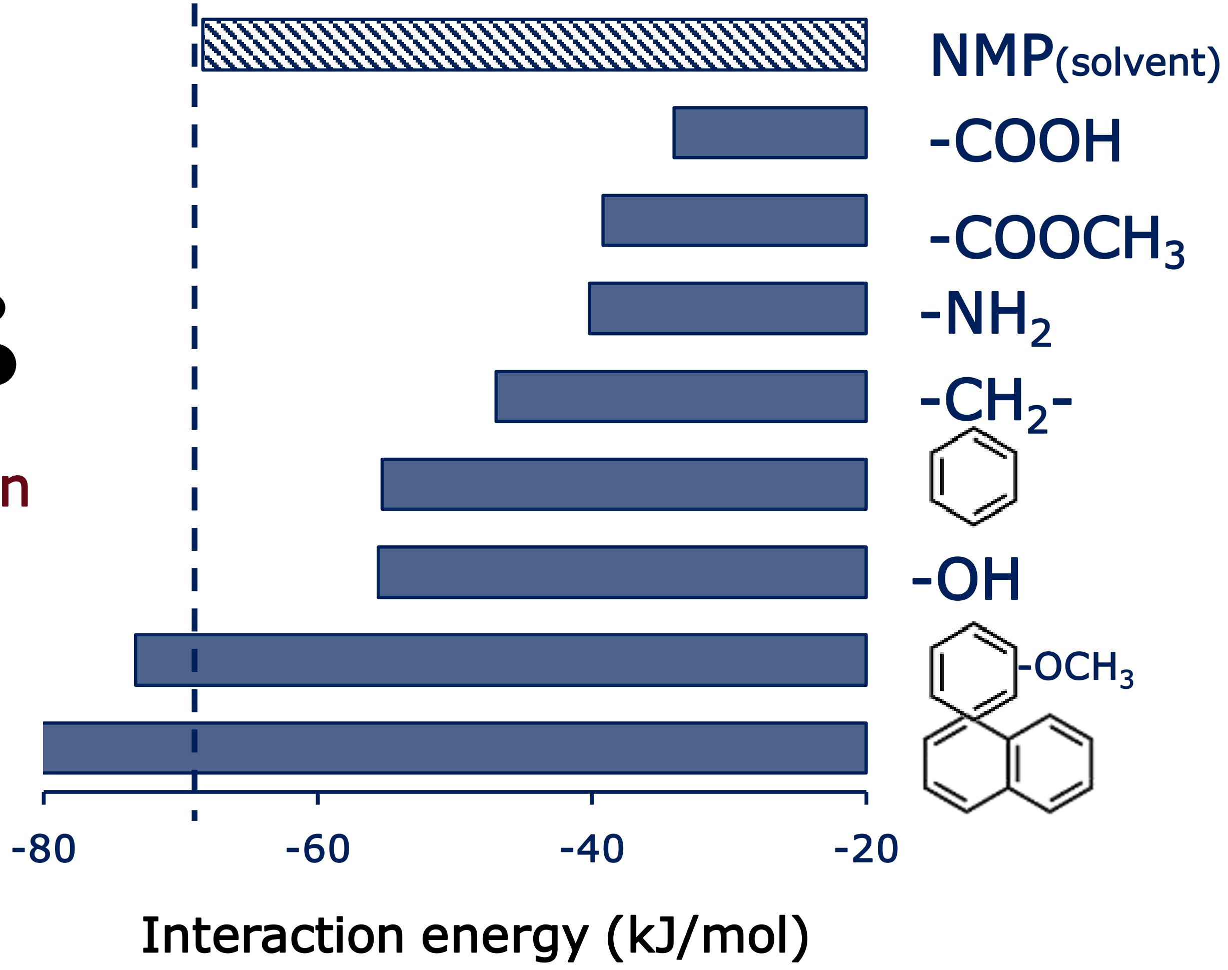
Conductive carbon surface
- ☐ Less oxidative site
- ☐ Graphite structure
- ☐ Hydrophobic flat plane

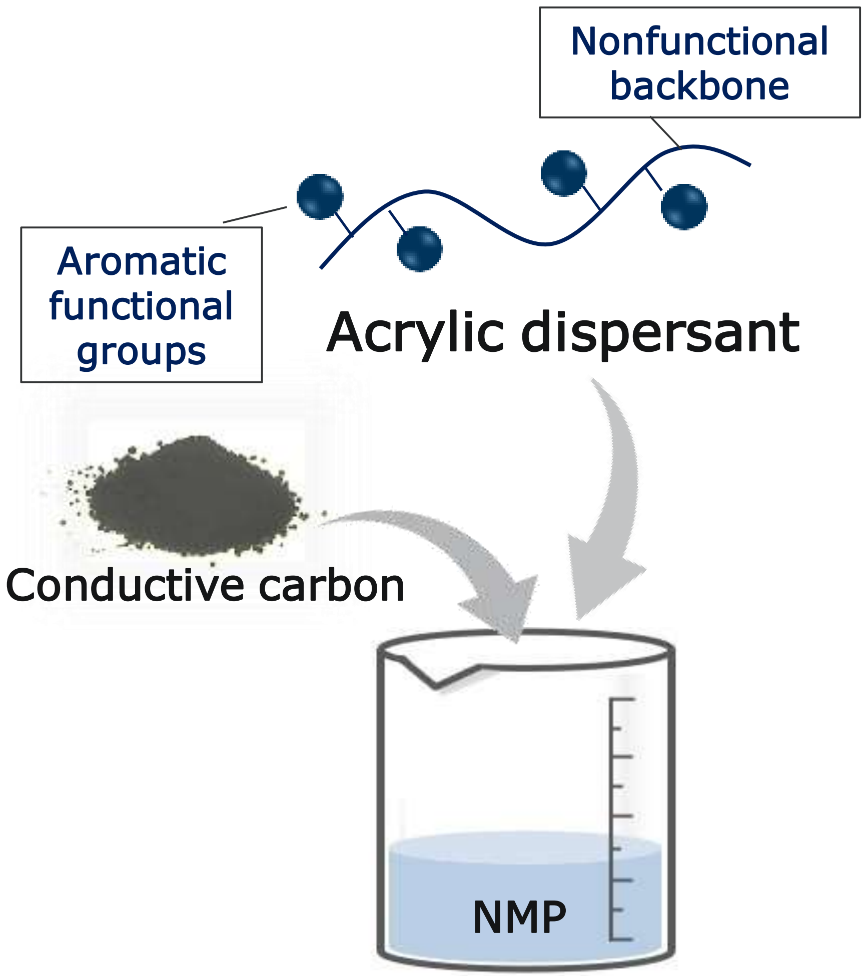


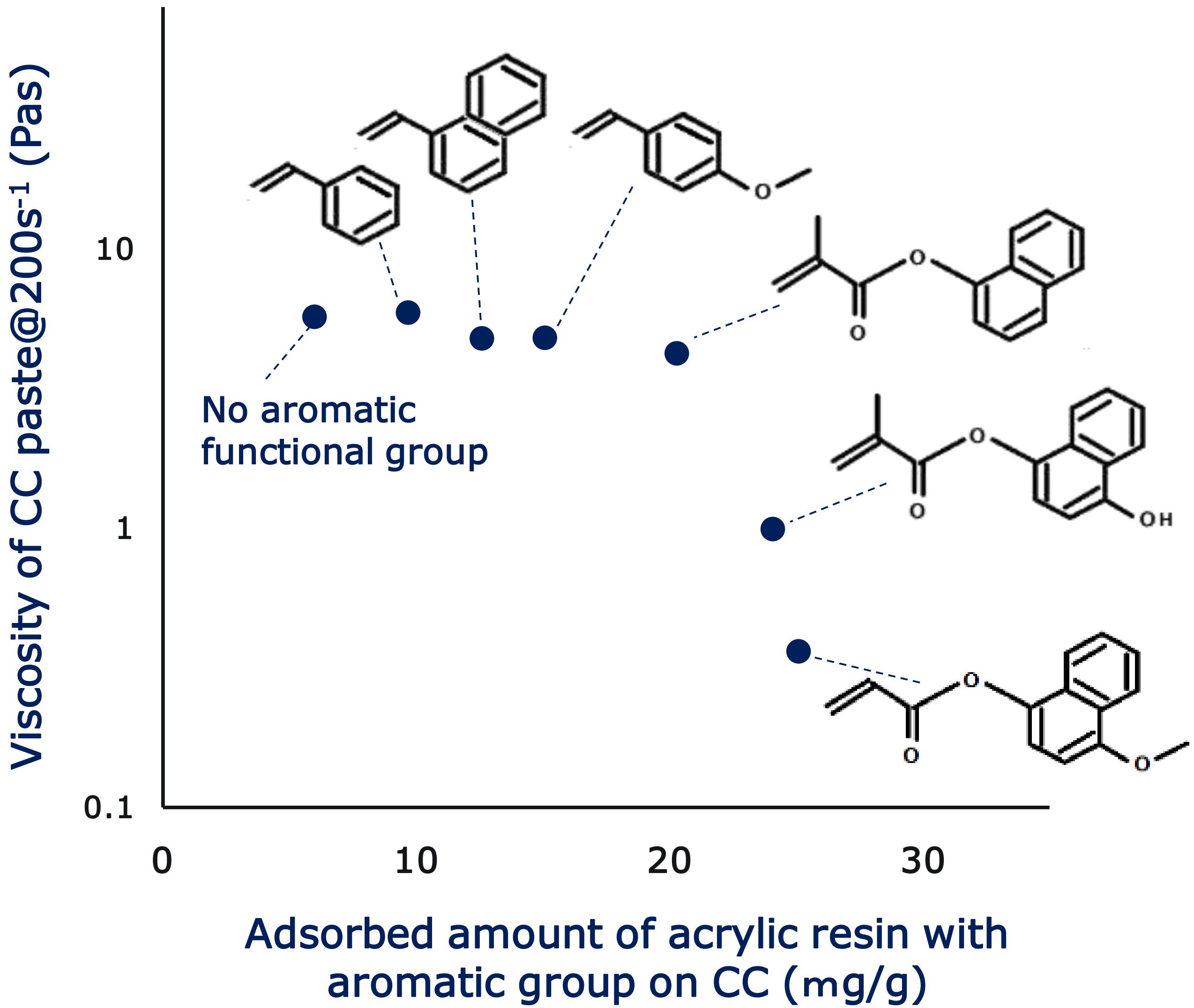
Interaction energy of functional groups onto graphite



Calculation basis set : ωB97X-D/6-31G(d)

Dispersant with aroma-ring and CC paste viscosity

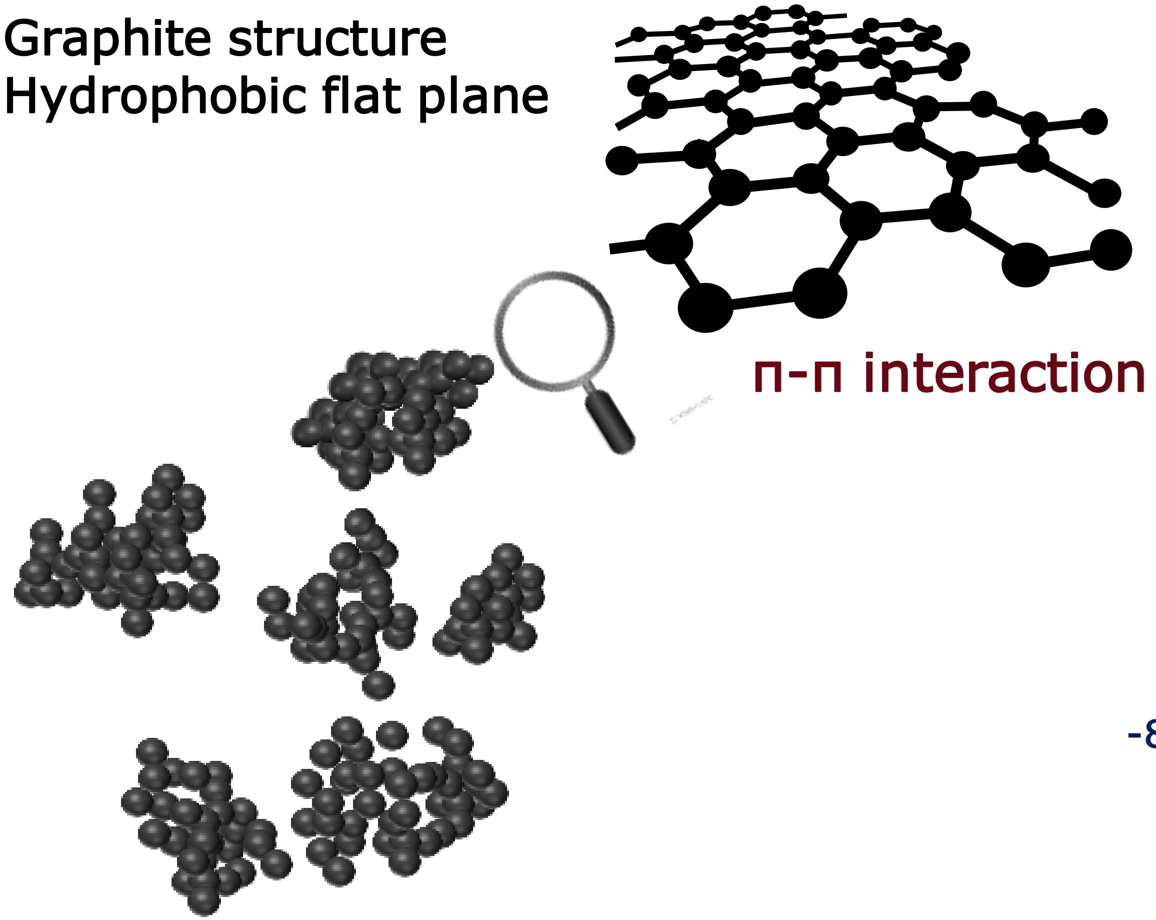




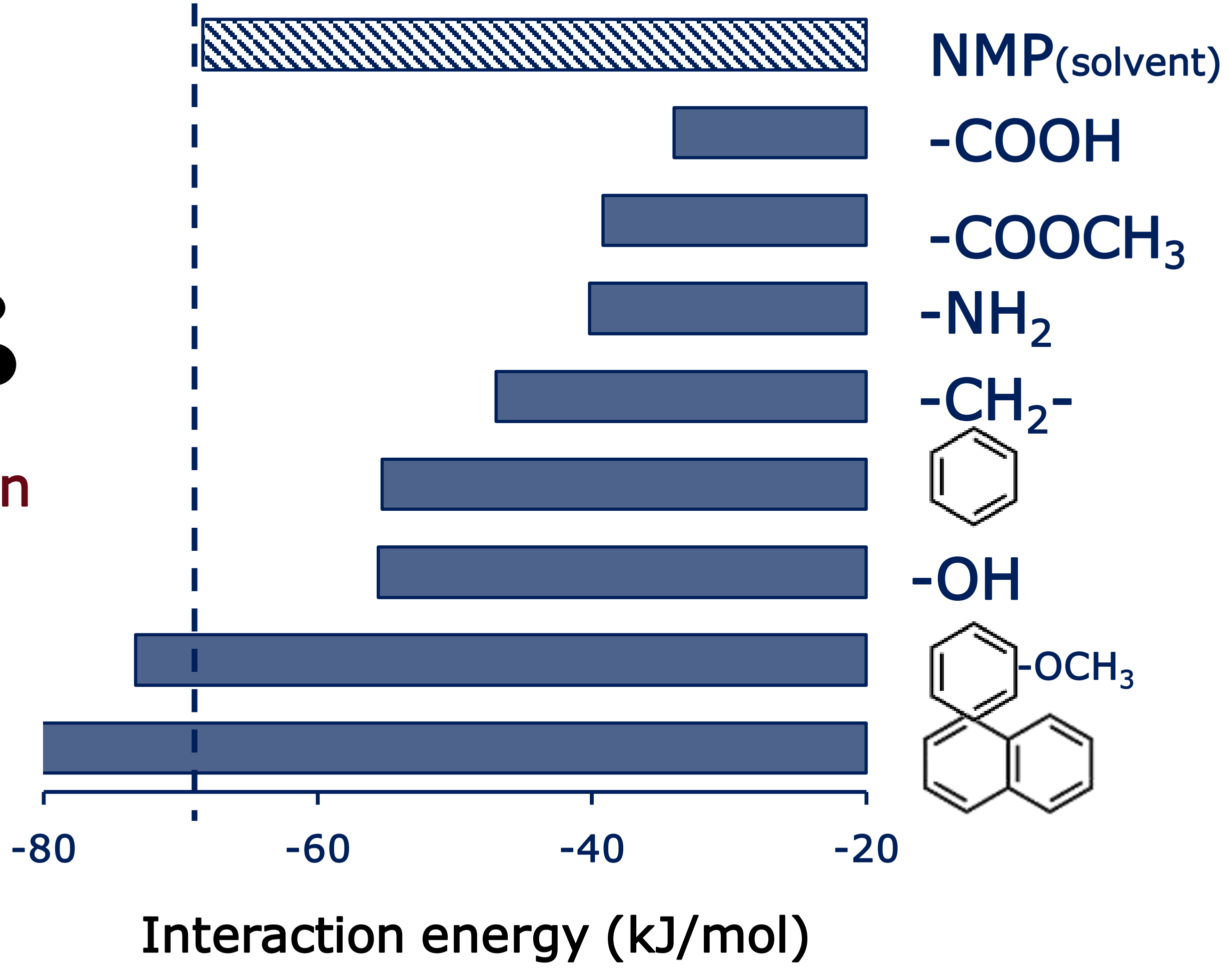
CC：Conductive carbon

Affinity of functional groups for graphite

Conductive carbon surface
- ☐ Less oxidative site
- ☐ Graphite structure
- ☐ Hydrophobic flat plane



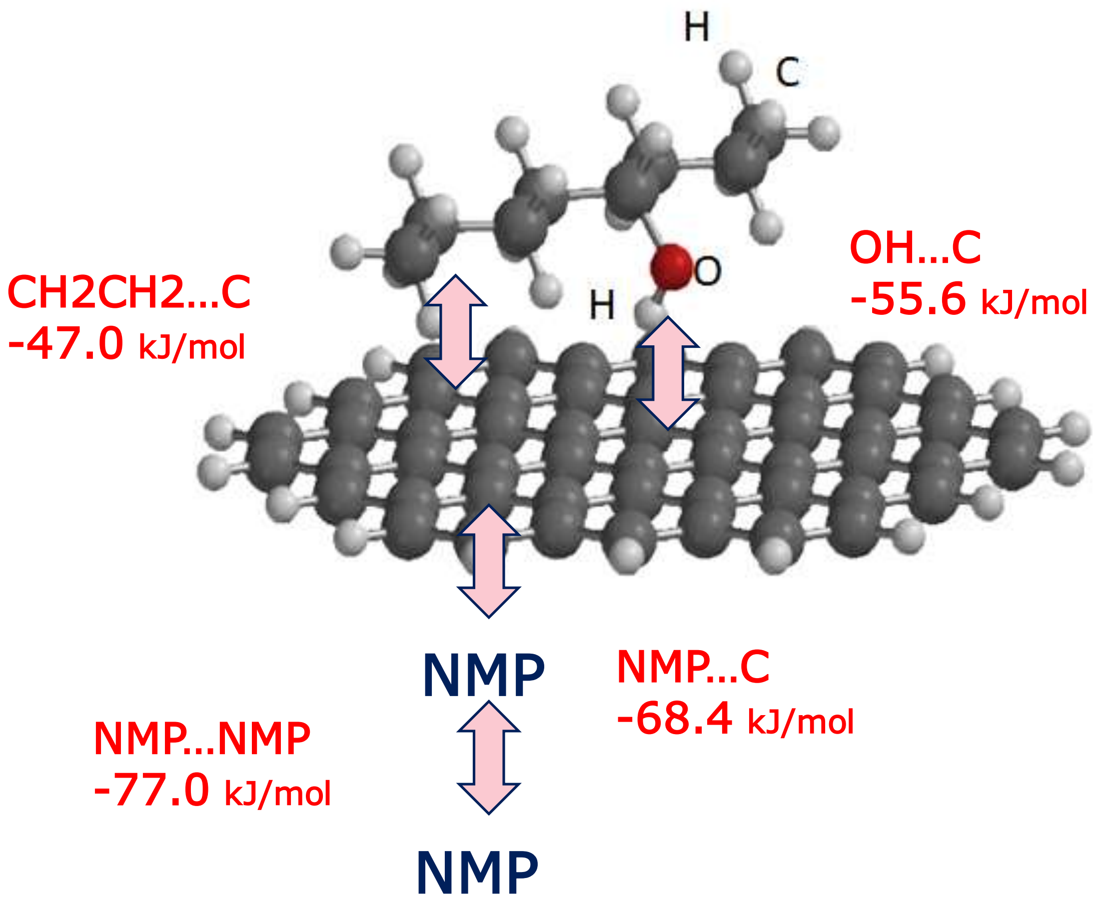
Interaction energy of functional groups onto graphite

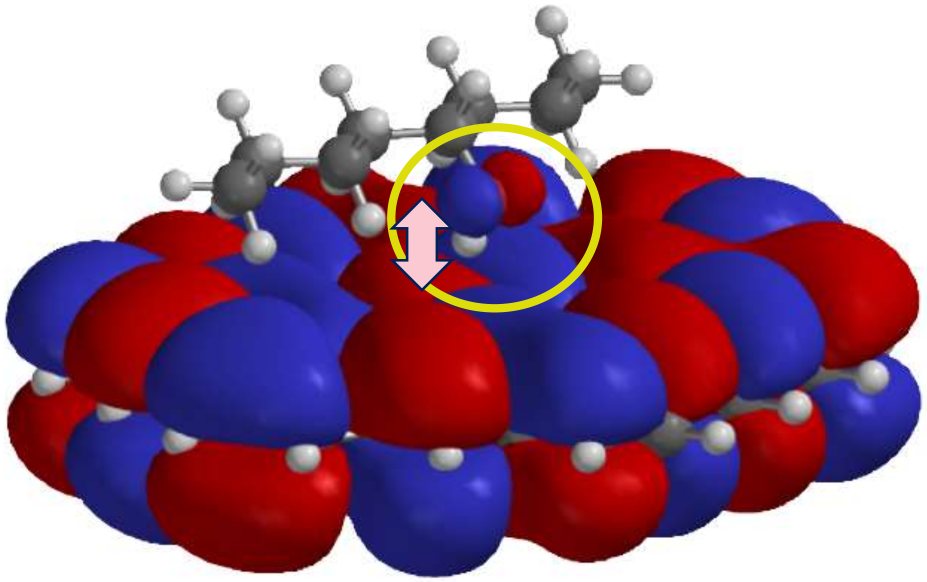


Calculation basis set : ωB97X-D/6-31G(d)

Interaction energy of OH and graphite surface

calculation basis set：ωB97X-D/6-31G(d)



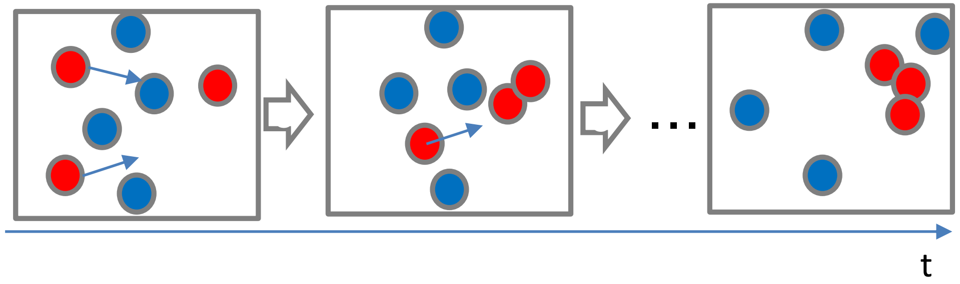


OH orbital interacted to
pi orbital on graphite surface

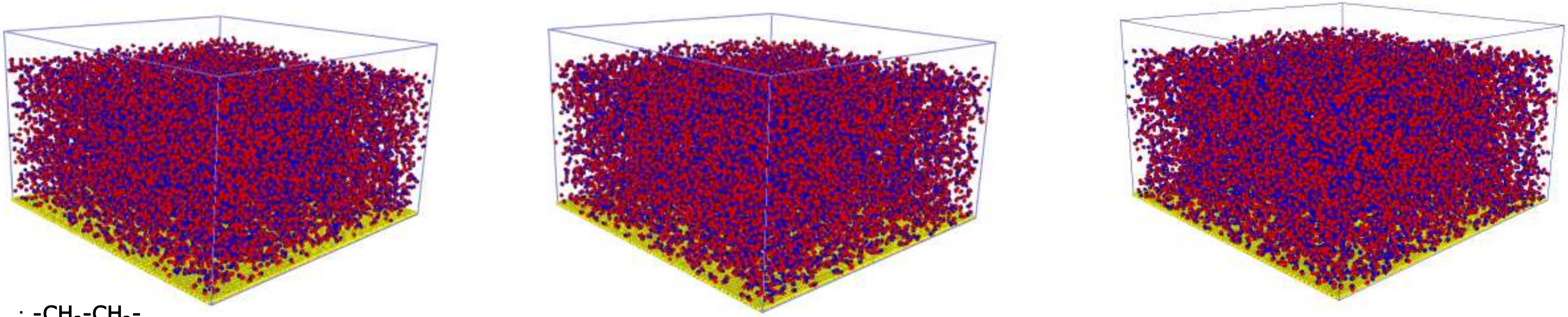
DPD calculation of Ethanol‘s state in NMP on graphite

Dissipative particle dynamics(DPD)
for minimum functional unit. CH3CH2-OH

【DPD】 Calculated position of sphere with force in step by step



Initial time progression (Calculation steps)



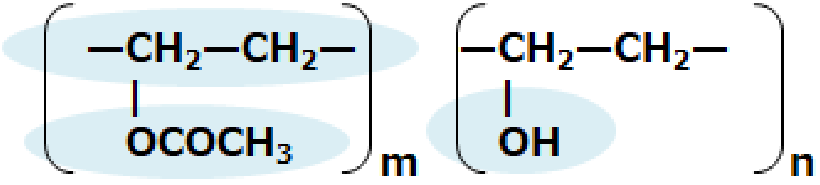
Blue : $-CH_2-CH_2-$
Red : -OH
NMP : not displayed

http://octa.com

Ethanol : adsorption onto graphite < thermal diffusion into NMP

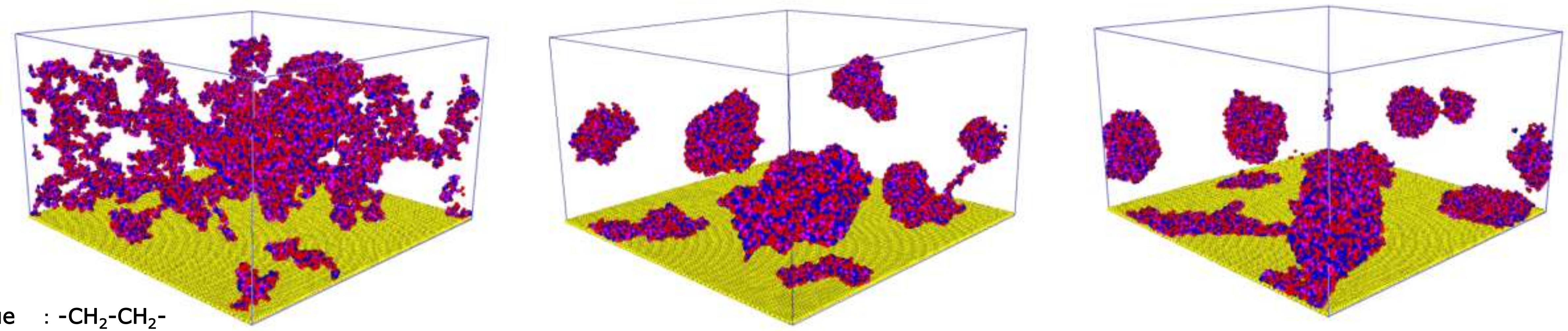
DPD calculation of PVA's state in NMP on graphite

Dissipative particle dynamics(DPD) for polymer unit. PVA(with -OH)



m=30 n=70

Initial → time progression (Calculation steps)



Blue : $-CH_2-CH_2-$
Red : -OH
Purple : -OCOCH3
NMP : not displayed

http://octa.com

PVA polymer : adsorption onto graphite ＞ thermal diffusion into NMP

DPD calculation of PVA's state in NMP on graphite

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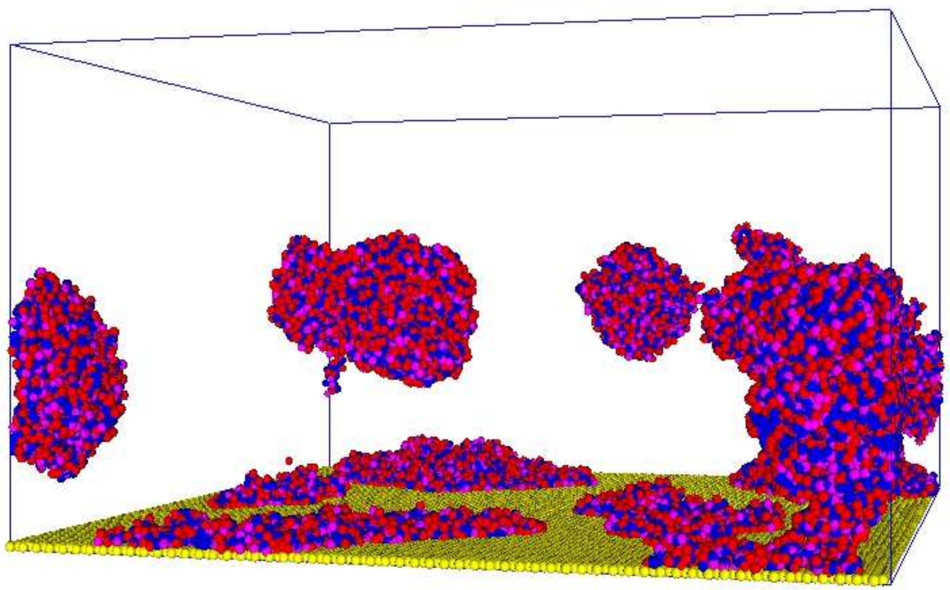
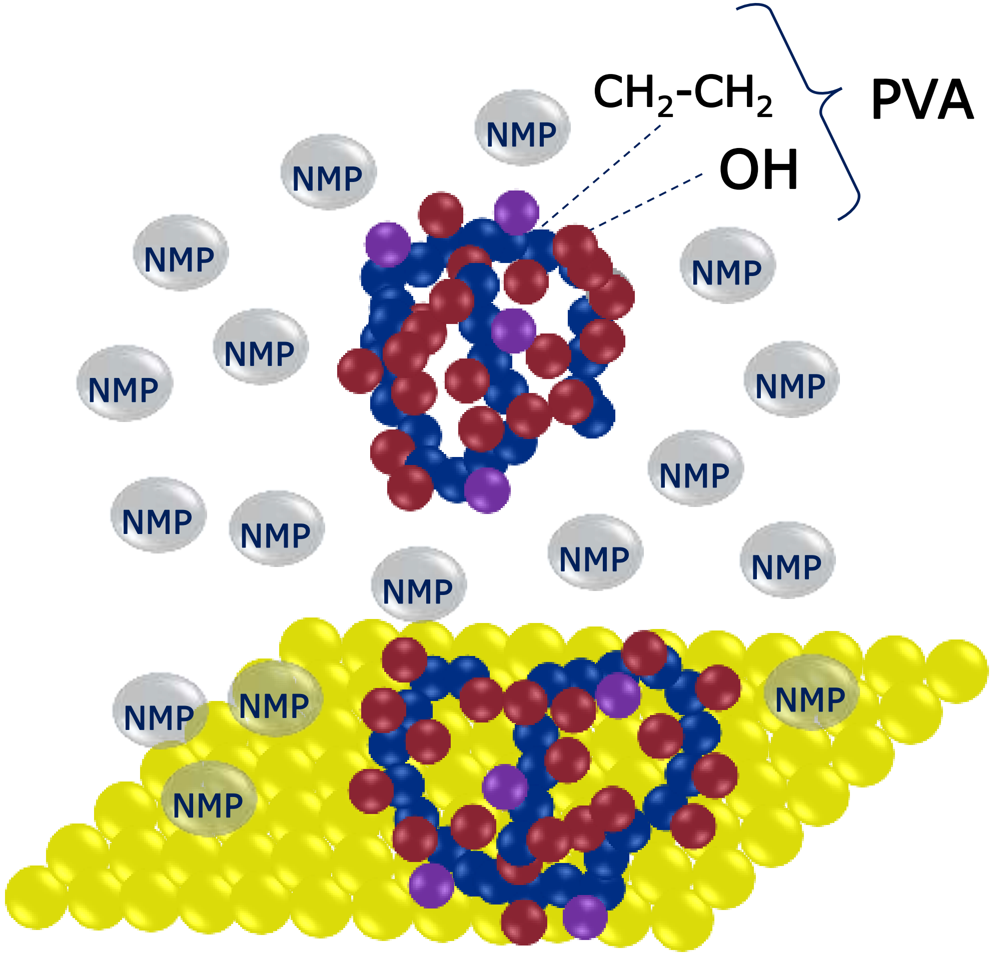
Dissipative particle dynamics(DPD) for polymer unit. PVA(with -OH)

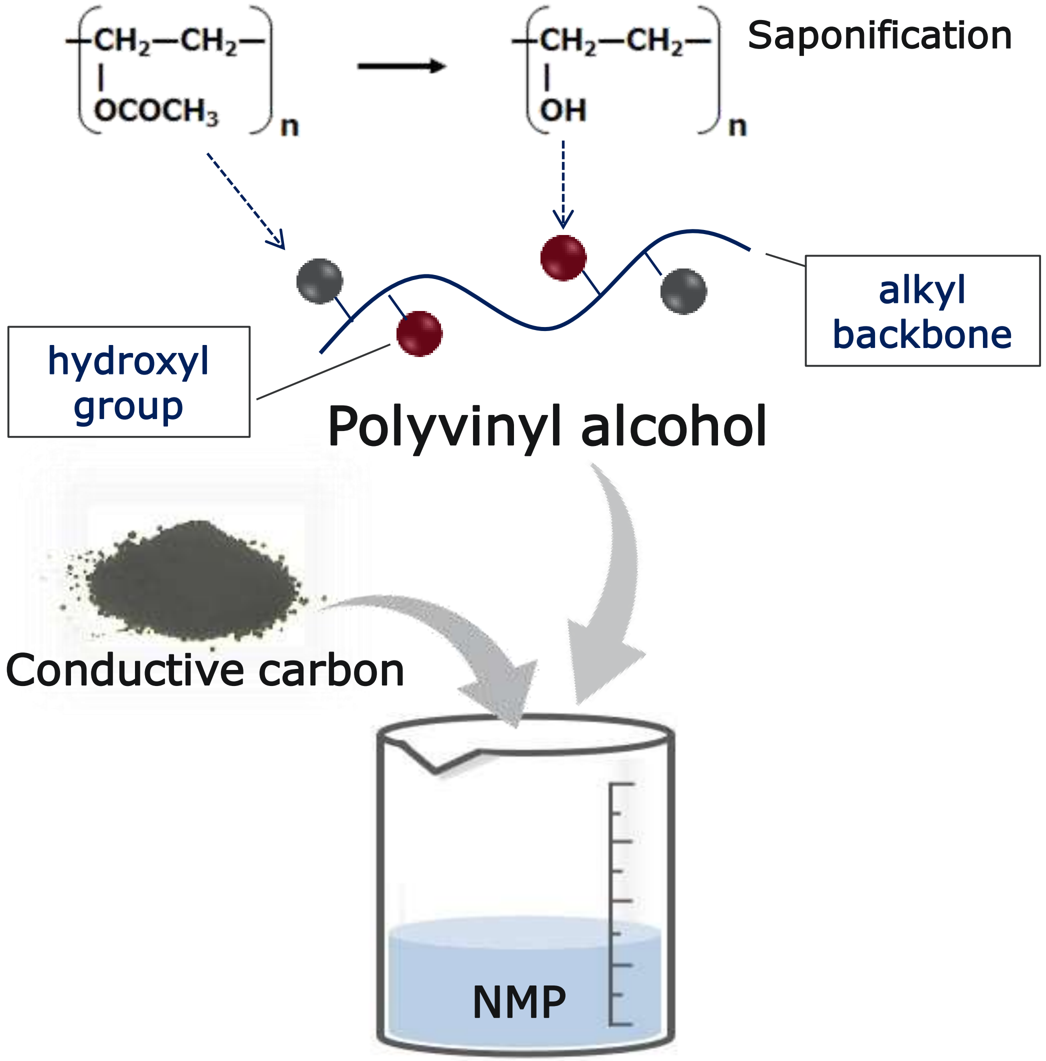


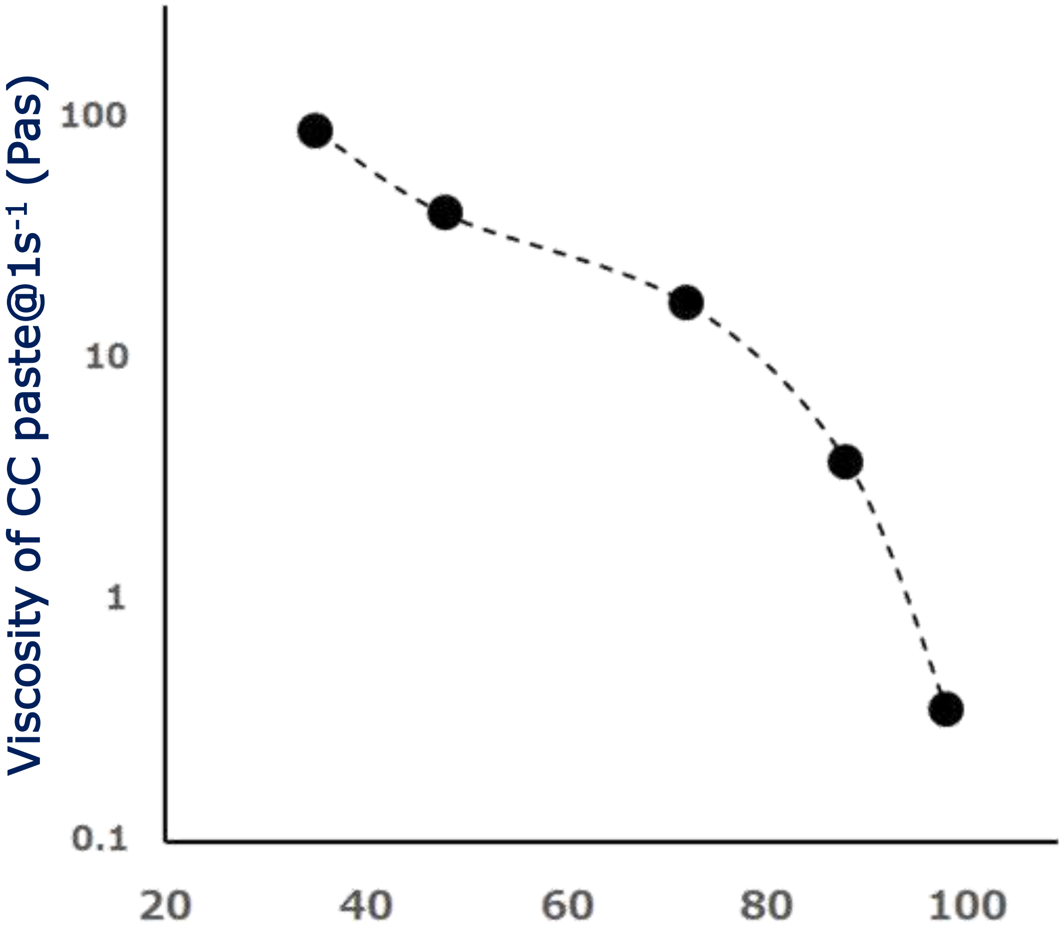
NMP: not displayed



Graphite
Conductive carbon surface

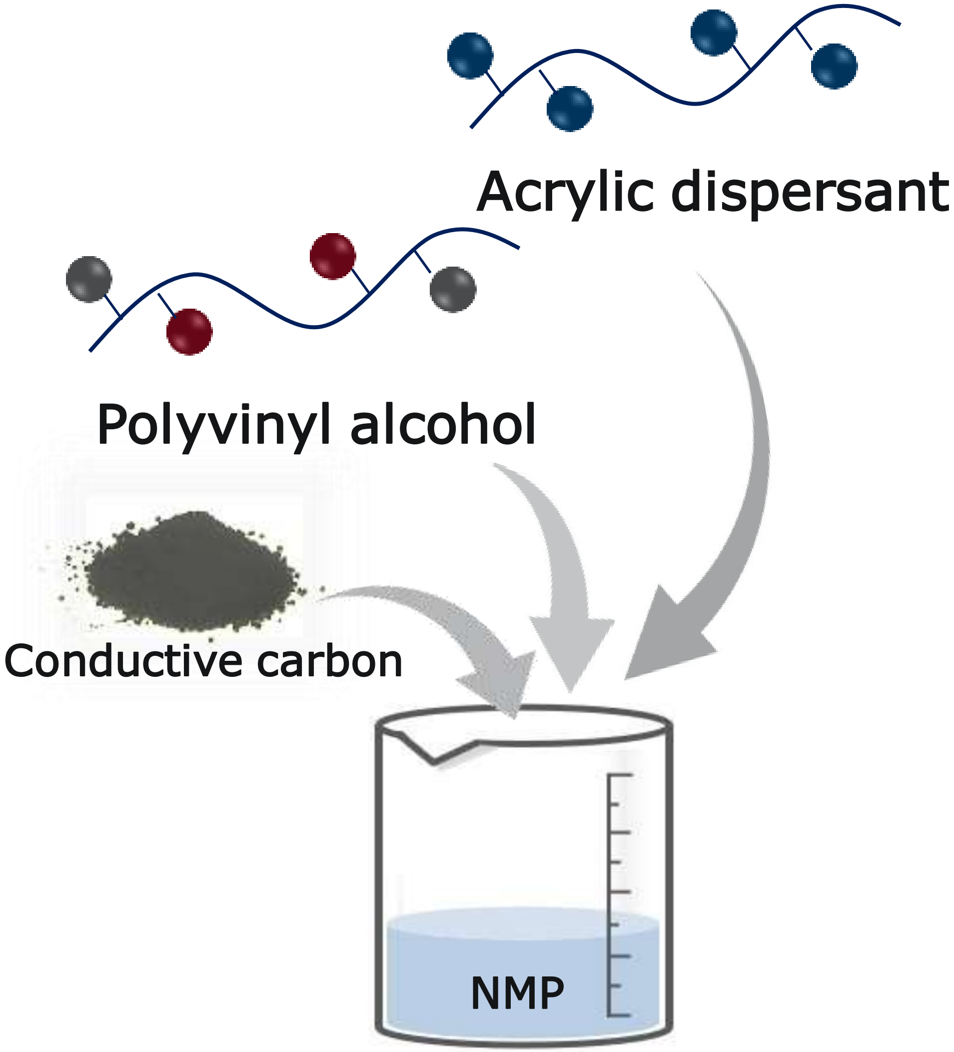
Dispersant with -OH and CC paste viscosity

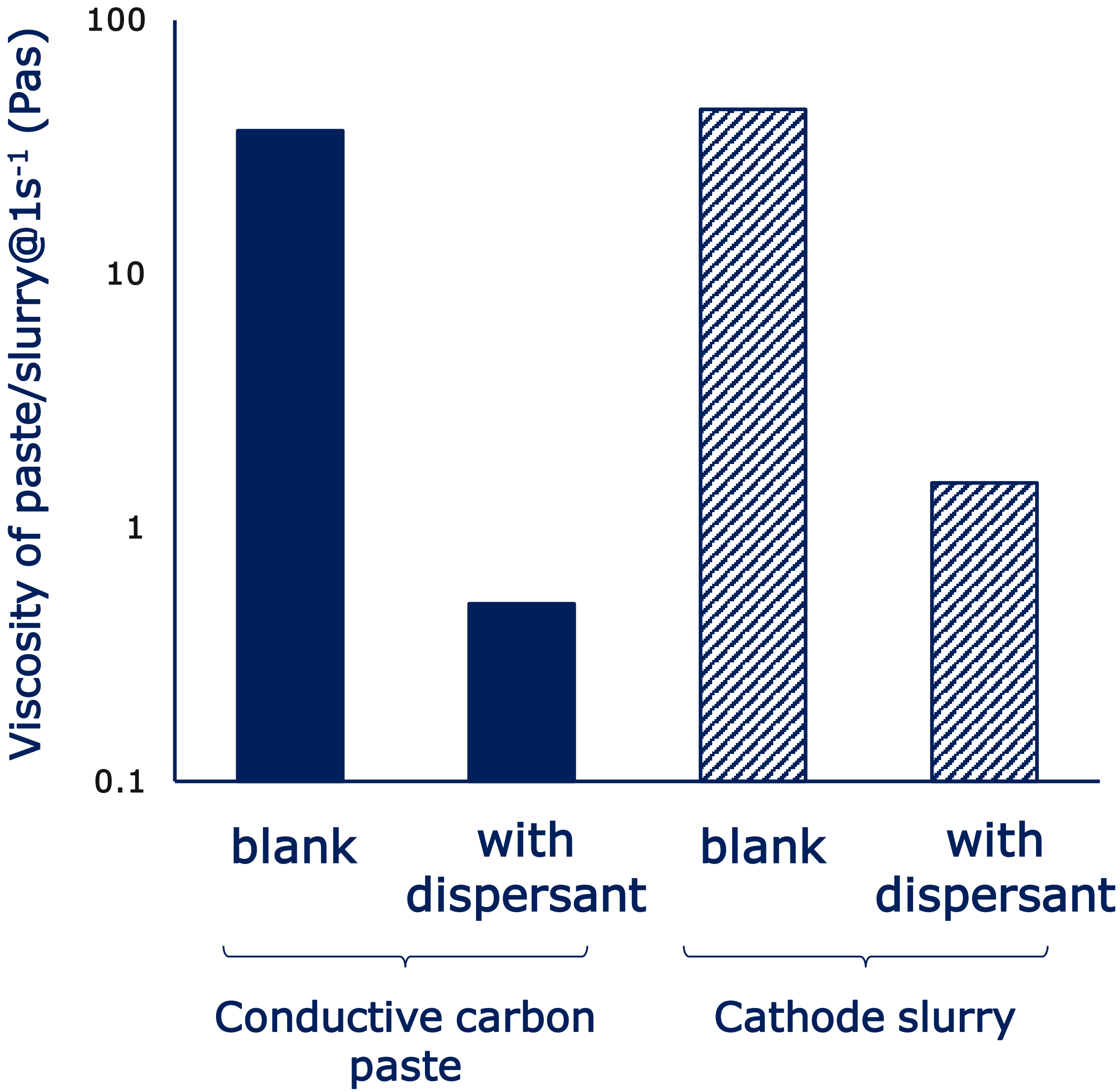




Saponification value of PVA(%)
: hydroxyl group content

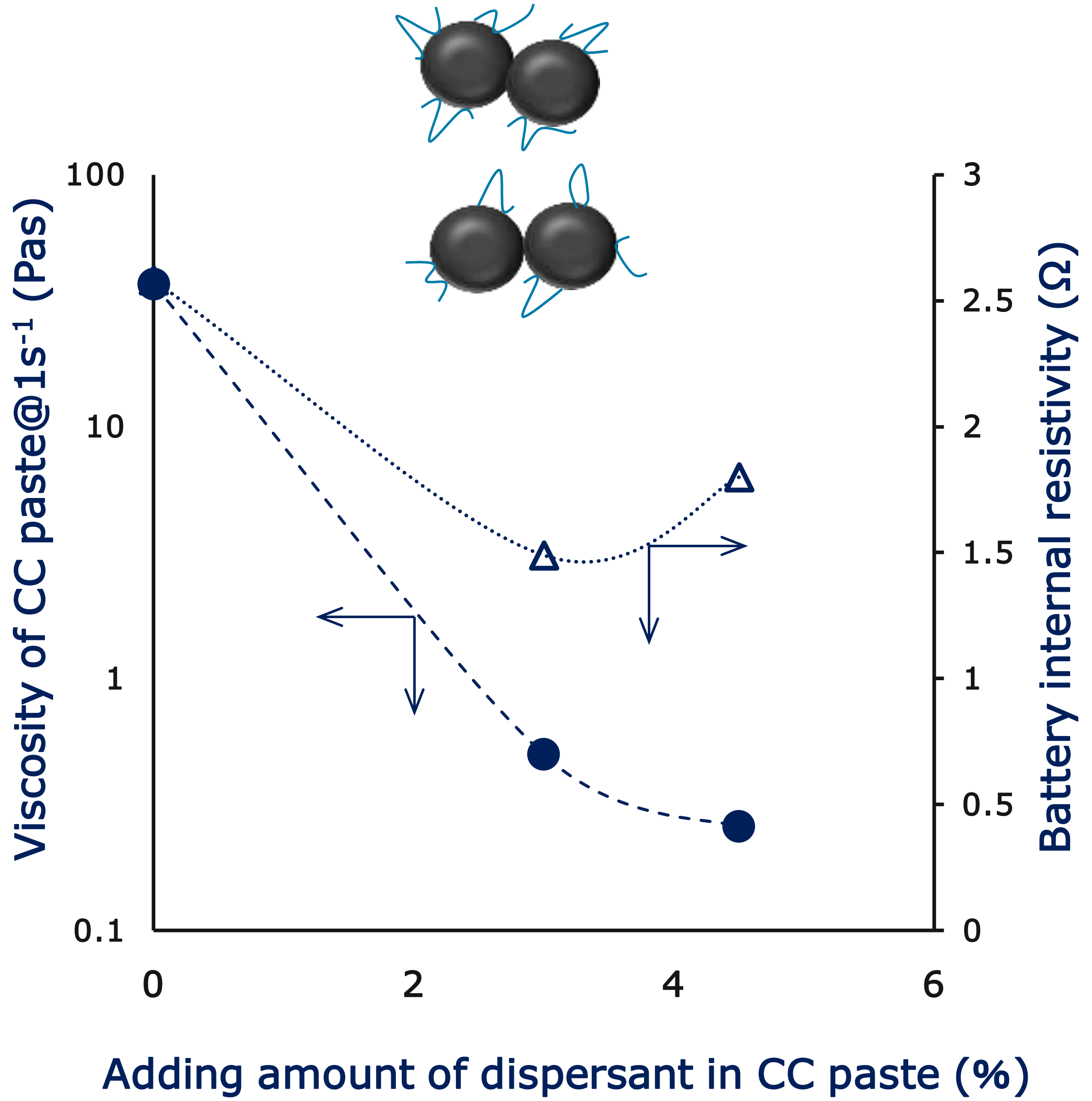
Combination of suitable dispersant and paste viscosity

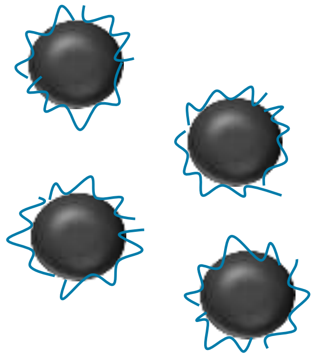




Amount of dispersant in CC paste and performance

Insufficient dispersing



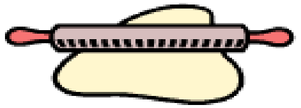


- ☐ Over dispersing
- ☐ Excessive addition of insulating dispersant

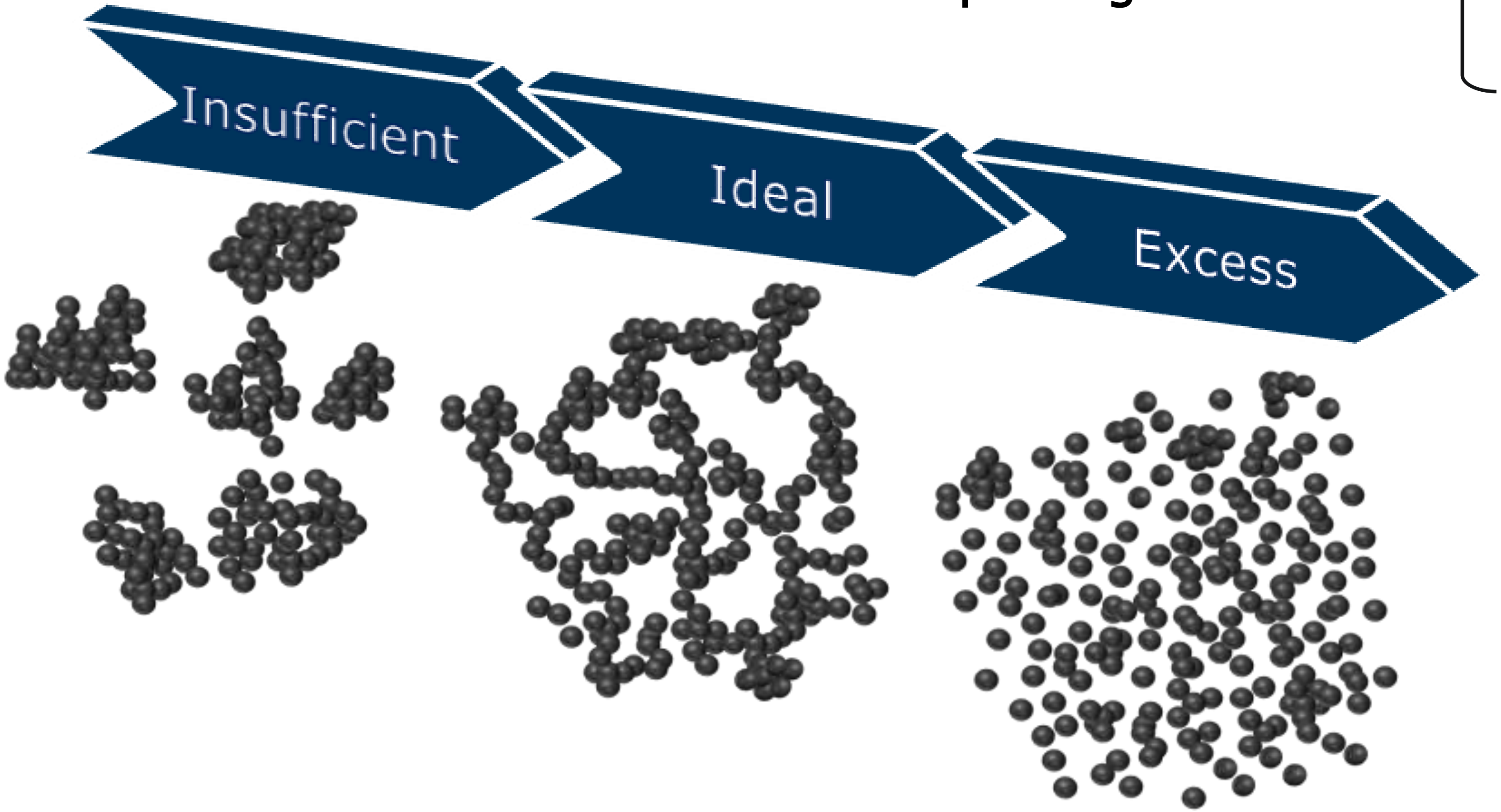
Optimization of dispersion process

Adjustment in degree of carbon dispersion

- Dispersing system
- Dispersing apparatus
- Dispersing condition

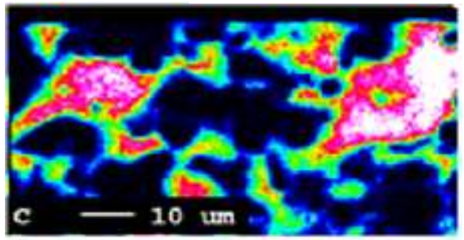
Smearing 

Smashing 

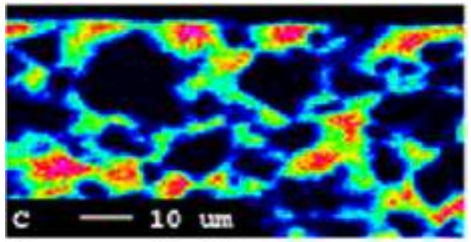


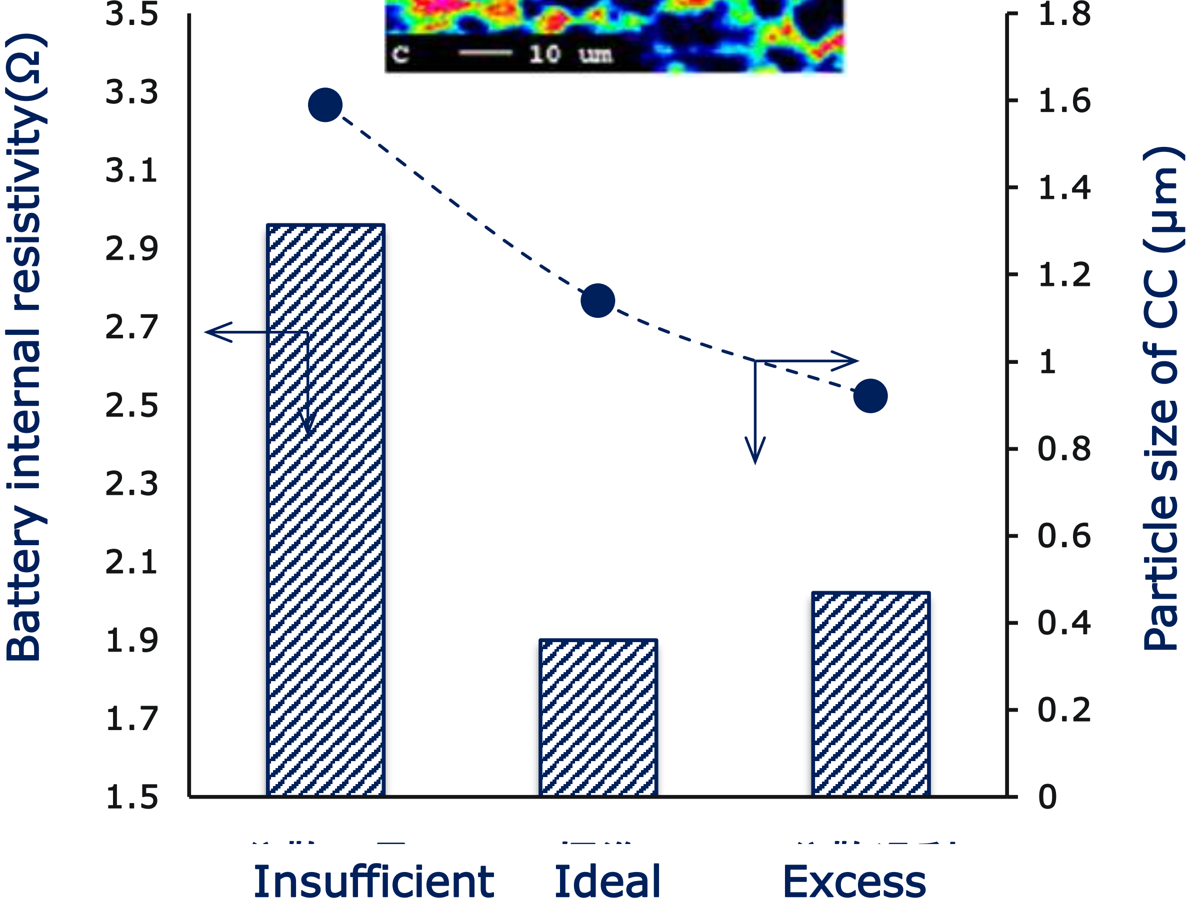
Dispersion progression of CC paste and performance

Cross-section image of cathode
EPMA C element mapping

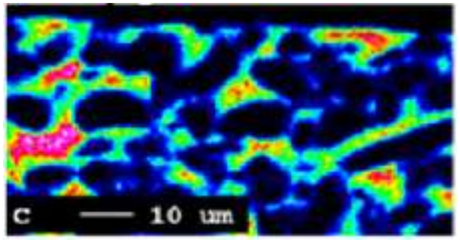


Carbon agglomeration
Disconnection of conductive paths





short Dispersing time long



Carbon isolation
Disconnection of conductive paths

Conclusion

KANSAI paint realized new conductive carbon paste
for LIB cathode coating

- by exploring suitable dispersants based on computational analysis
- by adjusting appropriate dispersing level

Future scenario of KANSAI's battery business

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2020 2021 2022 2024 2030

Acetylene carbon black (in NMP)

for HEV cathode

Smaller size

Completed!!

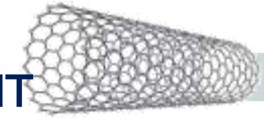
SOP

Carbon nanotube (in NMP)

for next gen. cathode

MW-CNT

Under development

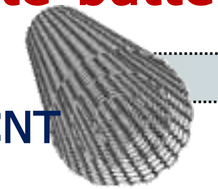


SW-CNT

Feasibility study

Carbon nanotube (in non-polar solvent)

for Solid-state-battery



MW-CNT

Feasibility study

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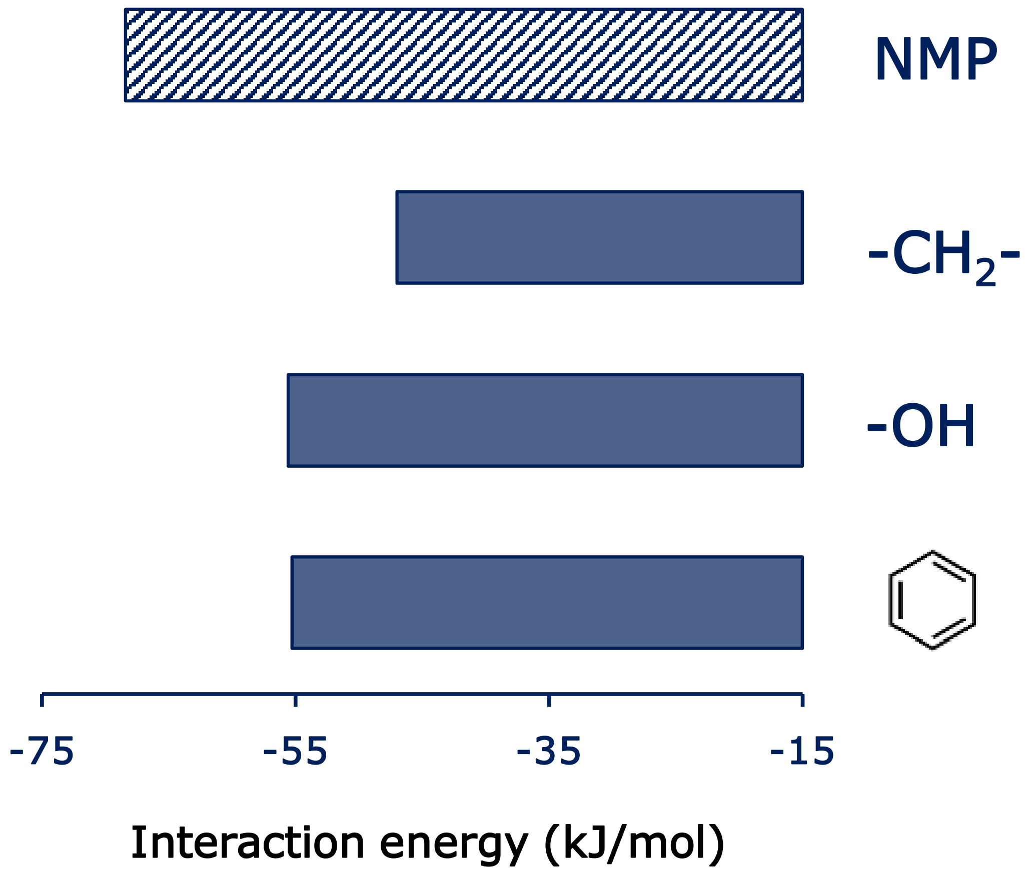
Affinity of functional groups vs NMP for graphite



Interaction energy with carbon surface

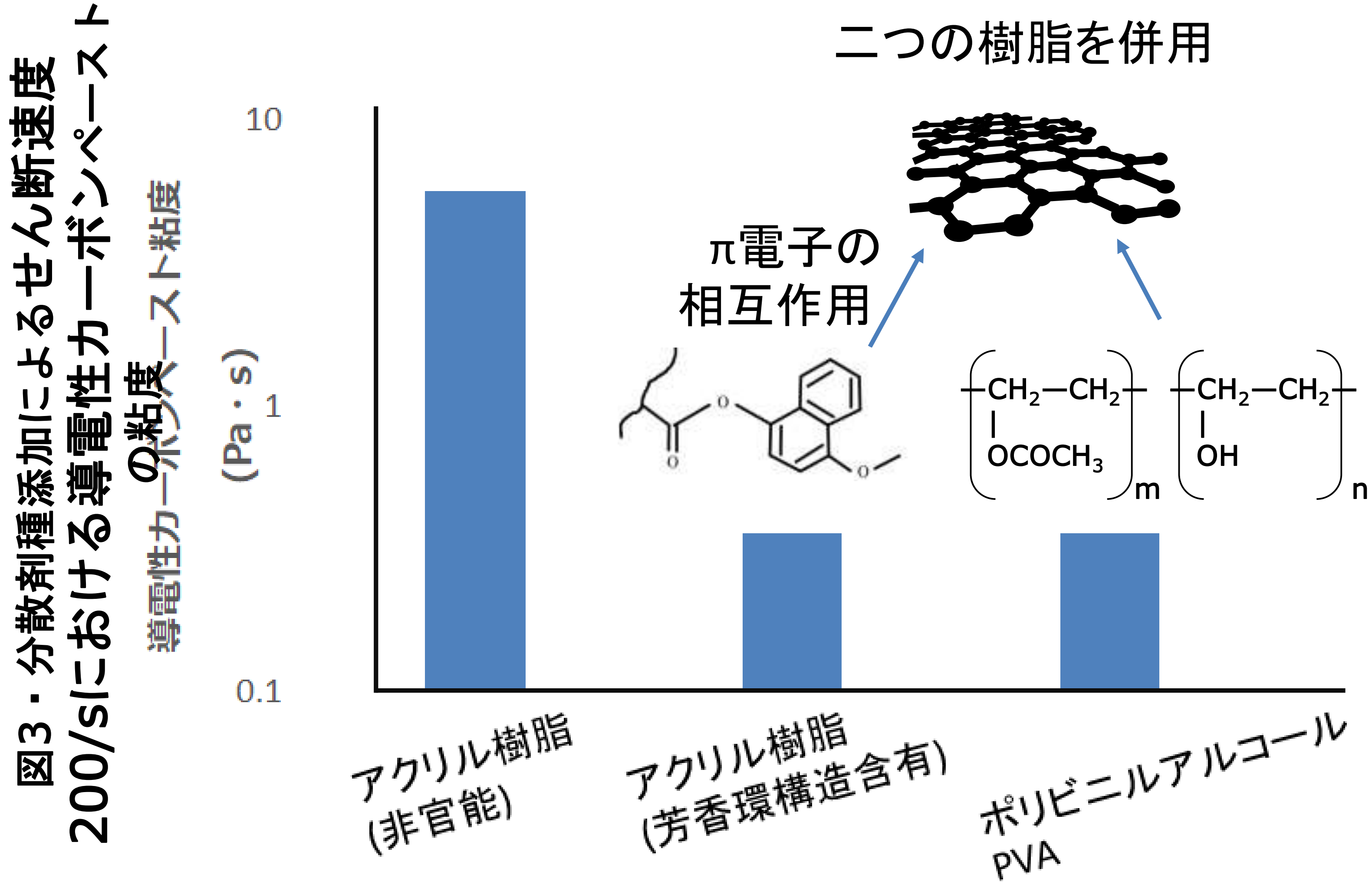
NMP (solvent) > Phenyl = OH

Calculation basis set : ωB97X-D/6-31G(d)

1. What is a good functional group for dispersing

Formulation design

二つの樹脂を併用



芳香環構造だけでなく、PVAも相互作用により吸着・分散効果があることがわかった。

1. Optimizing the dispersing process

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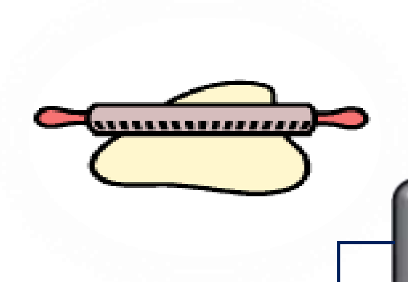
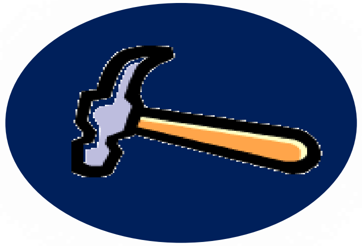


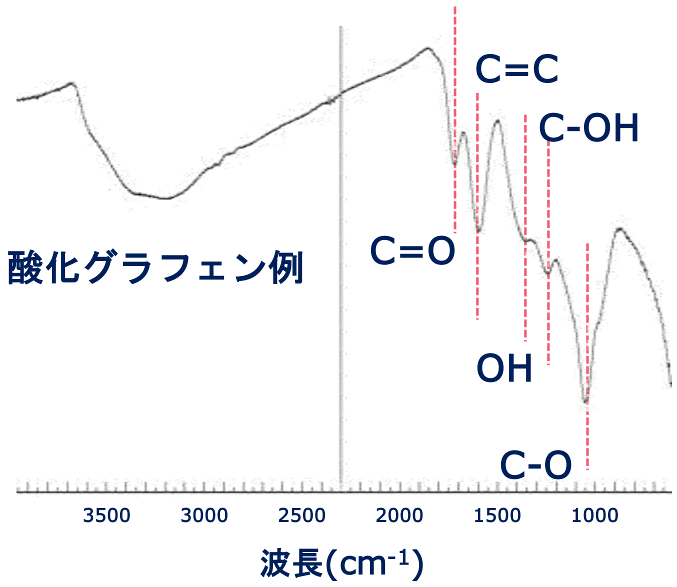
Dispersing system

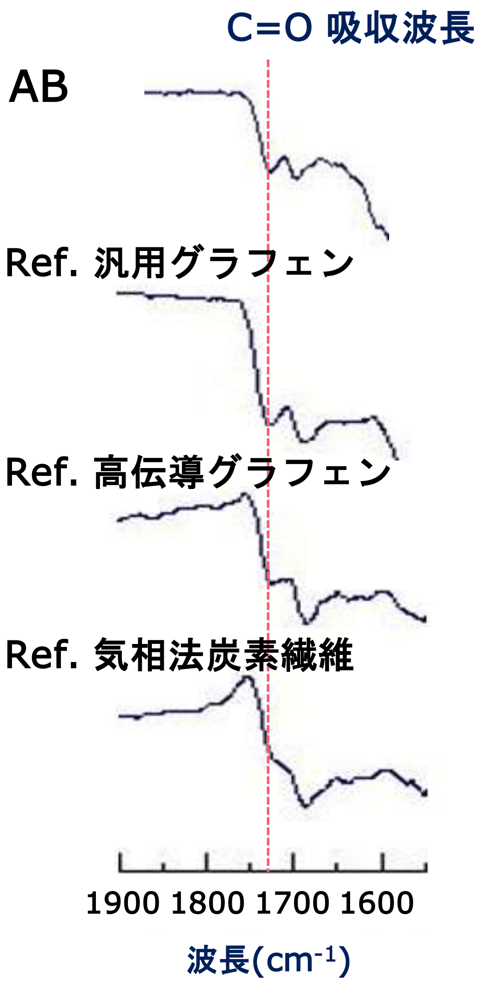
- Smearing
  - Roll mill
  - Biaxial kneader
  - Planetary mixer
  - Homogenizer
  - Disperser …
- Smashing
  - Beads mill
  - Ball mill …

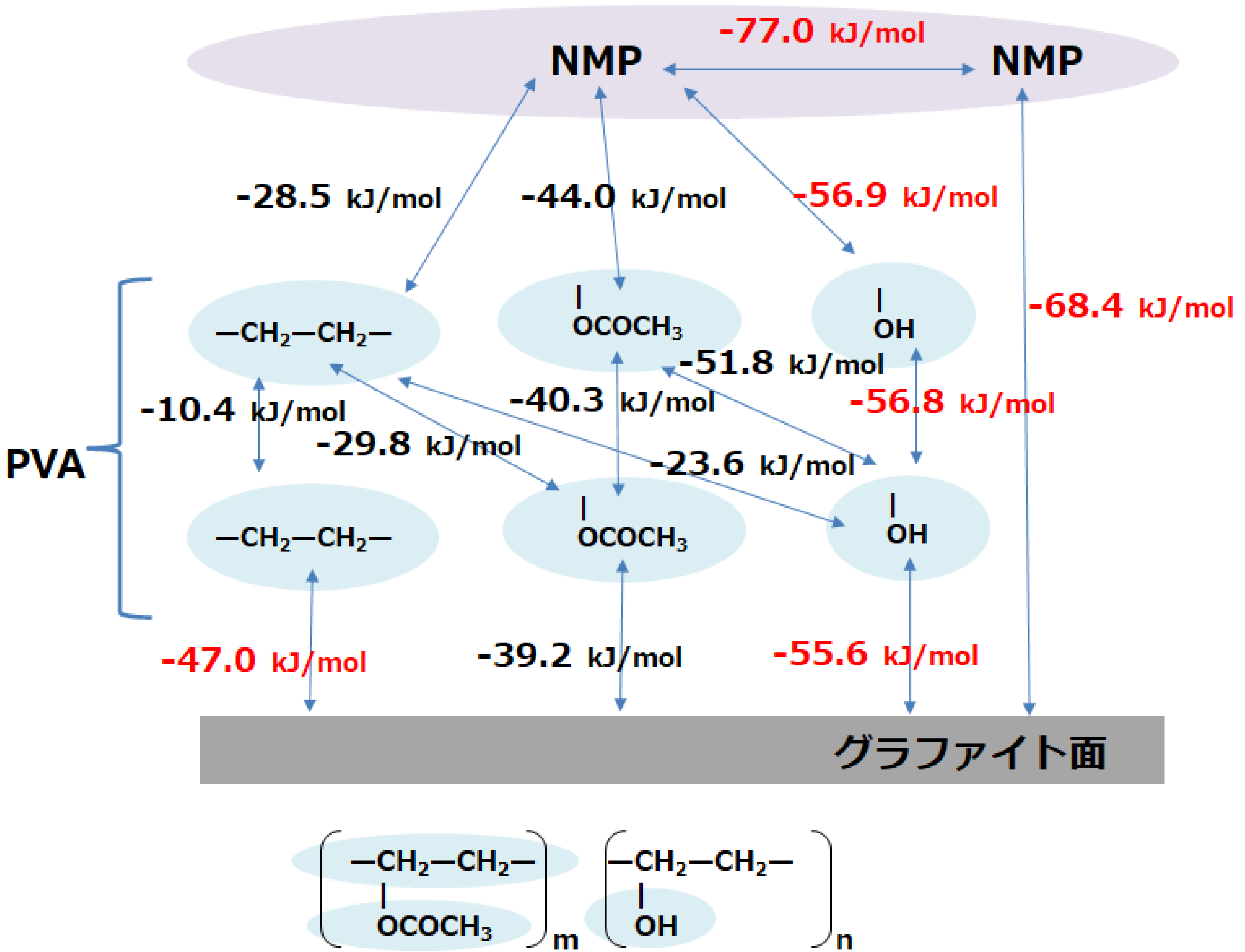


KANSAI has various dispersing methods

Why dose the OH group interact carbon surface?

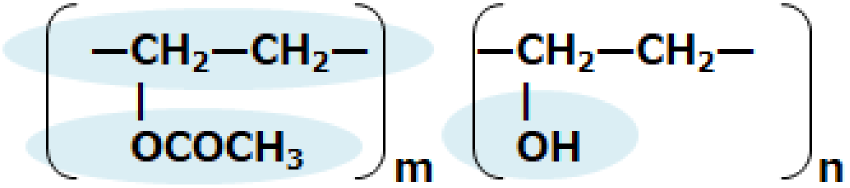

C=C
C-OH
C=O
OH
C-O
酸化グラフェン例
3500
3000
2500
2000
1500
1000
波長(cm-1)


C=O 吸収波長
AB
Ref. 汎用グラフェン
Ref. 高伝導グラフェン
Ref. 気相法炭素繊維
1900 1800 1700 1600
波長(cm-1)

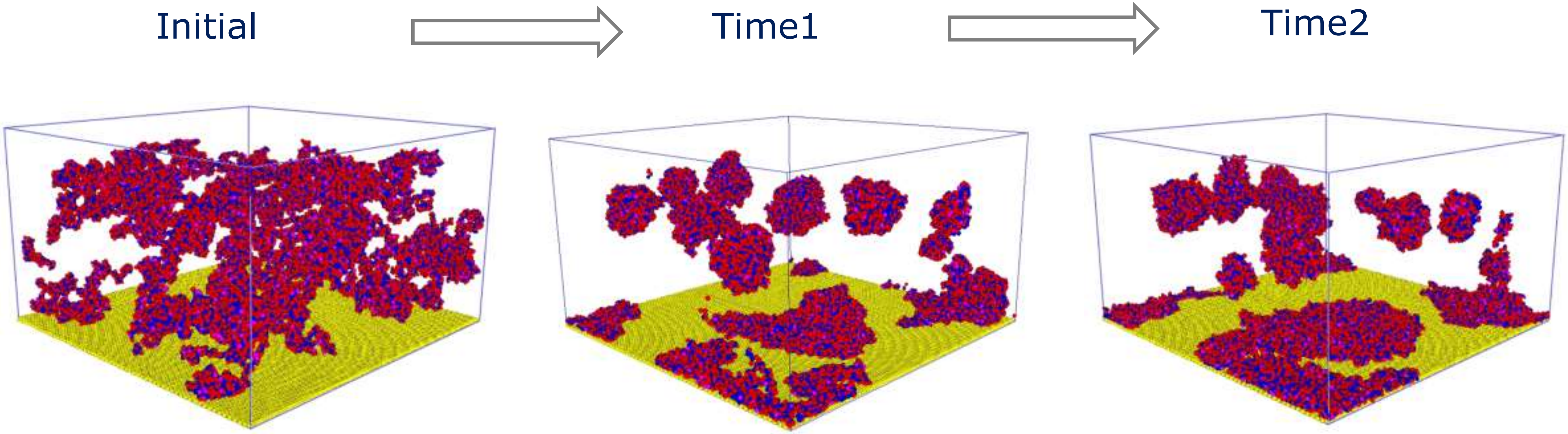

NMP
-77.0 kJ/mol
NMP
-28.5 kJ/mol
-44.0 kJ/mol
-56.9 kJ/mol
-68.4 kJ/mol
PVA
—CH₂—CH₂—
OCOCH₃
OH
-51.8 kJ/mol
-10.4 kJ/mol
-40.3 kJ/mol
-56.8 kJ/mol
-29.8 kJ/mol
-23.6 kJ/mol
—CH₂—CH₂—
OCOCH₃
OH
-47.0 kJ/mol
-39.2 kJ/mol
-55.6 kJ/mol
グラファイト面
—CH₂—CH₂—
OCOCH₃
m
—CH₂—CH₂—
OH
n

Formulation design

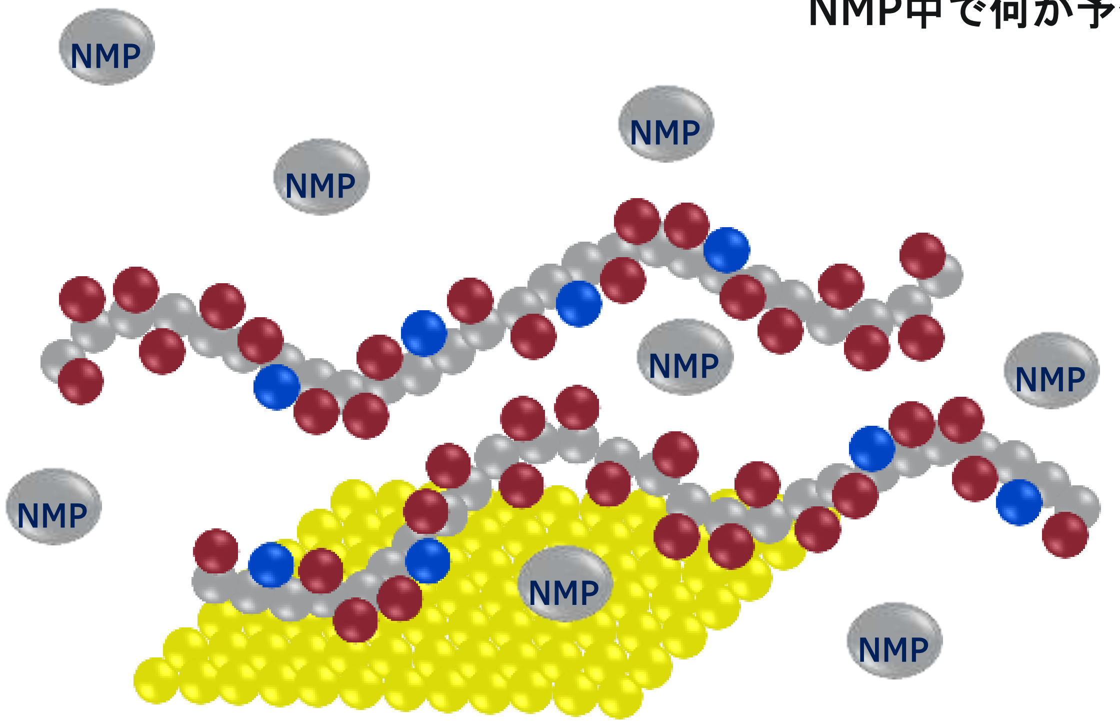
DPDの結果

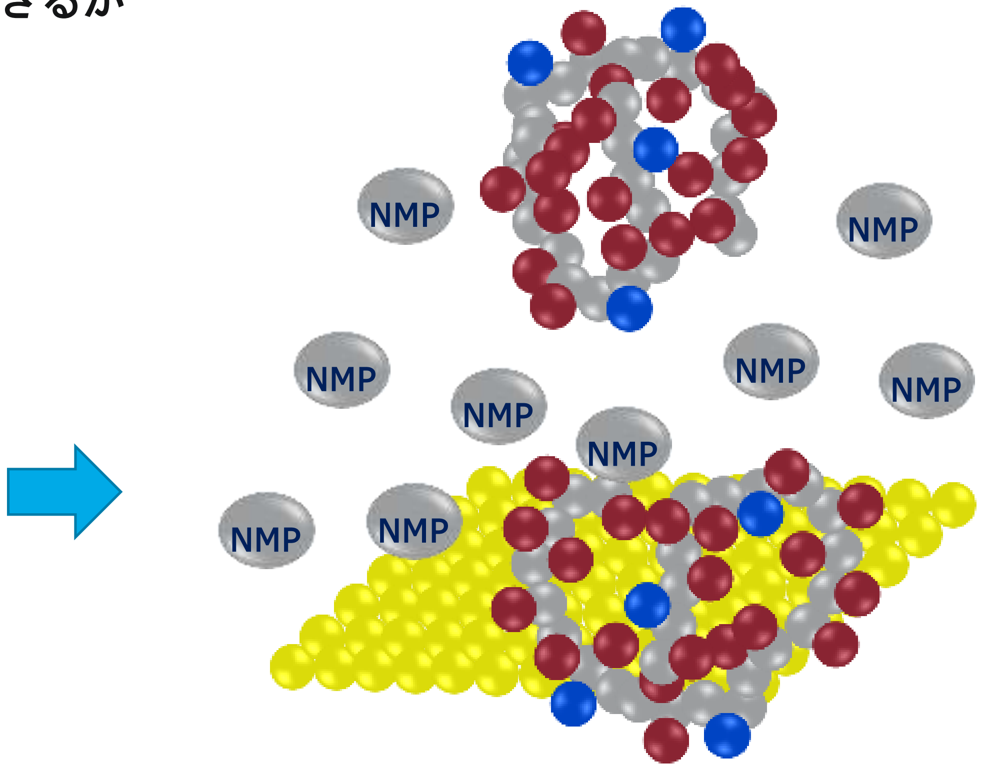


m=11 n=89



OHとグラファイトの相互作用の結果
NMP中で何が予想できるか





DPDシミュレーションで検討