

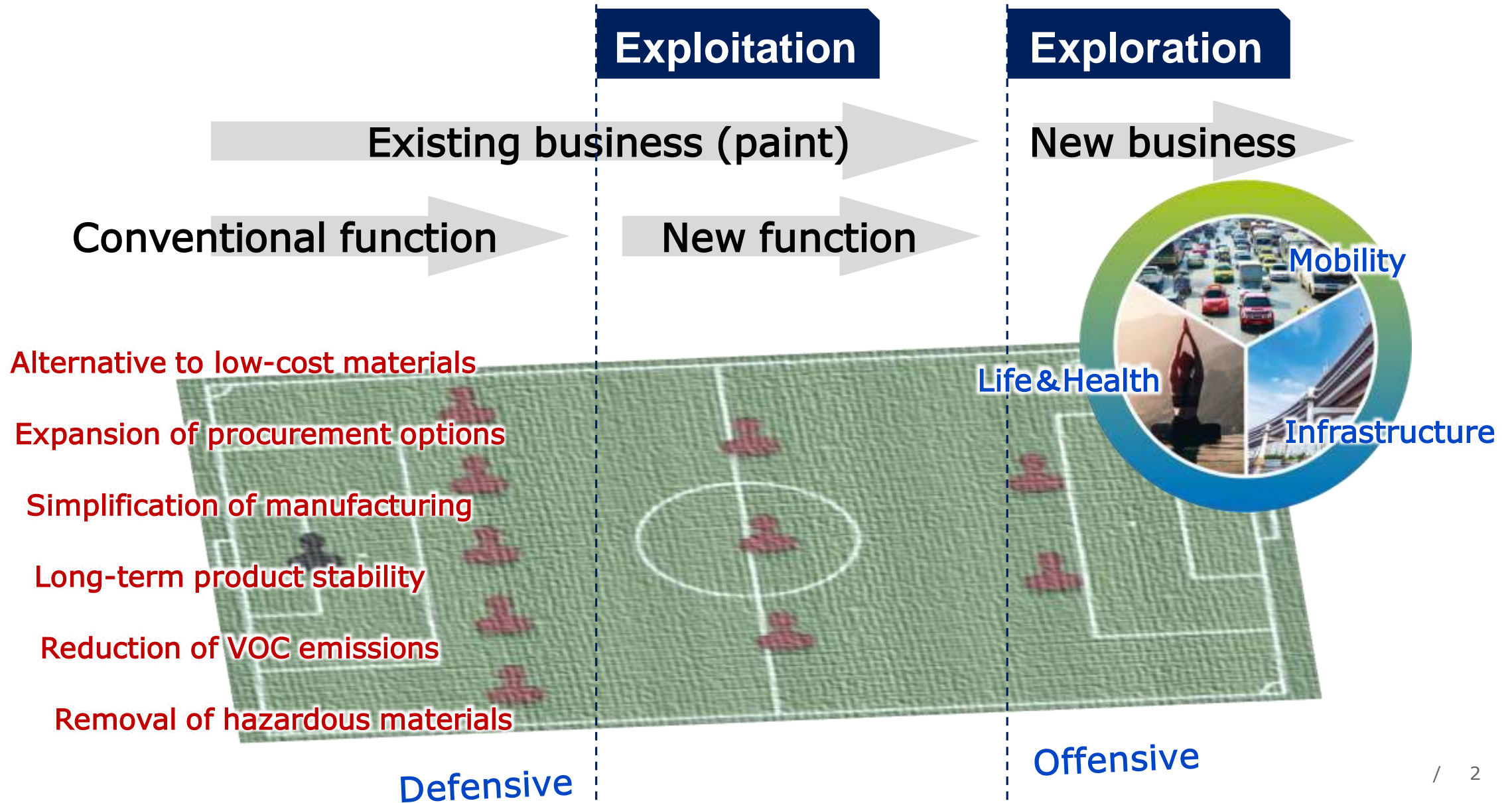


Development of conductive assistant slurry for lithium-ion batteries based on coating technologies

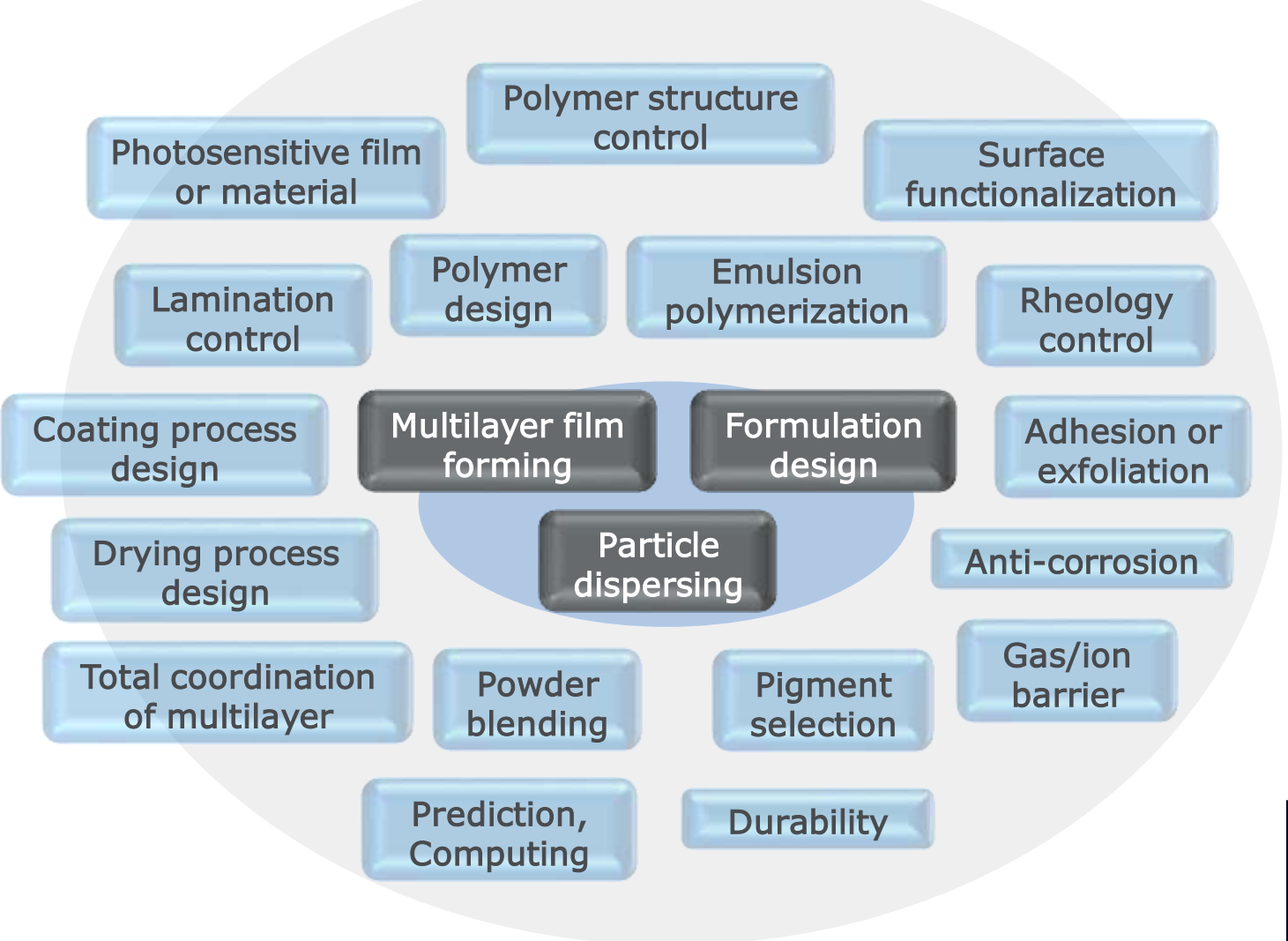
Kansai Paint Co.,Ltd.
Corporate Research and Development
Research and Development Division

Atsunao HIWARA
Chihiro NAGANO

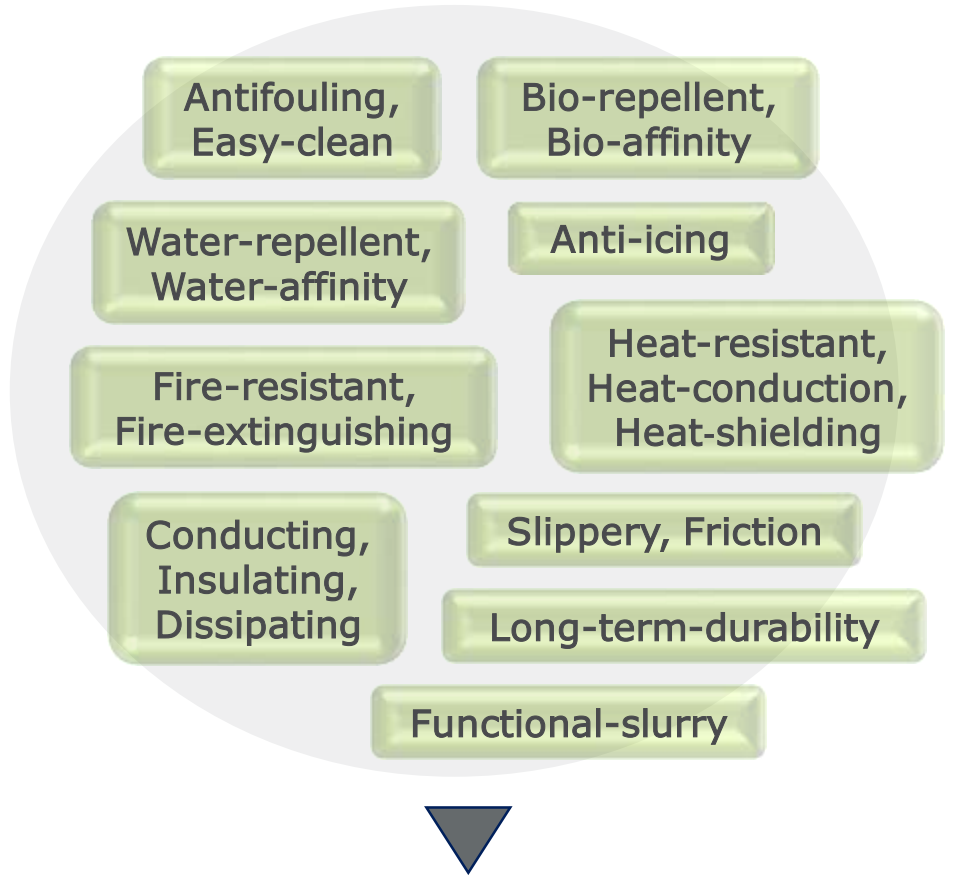
Ambidexterity strategy in KANSAI paint



Core technologies



Potential value propositions



Exploration of potential market or new business frontier

Potential entry opportunities in LIB industry

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

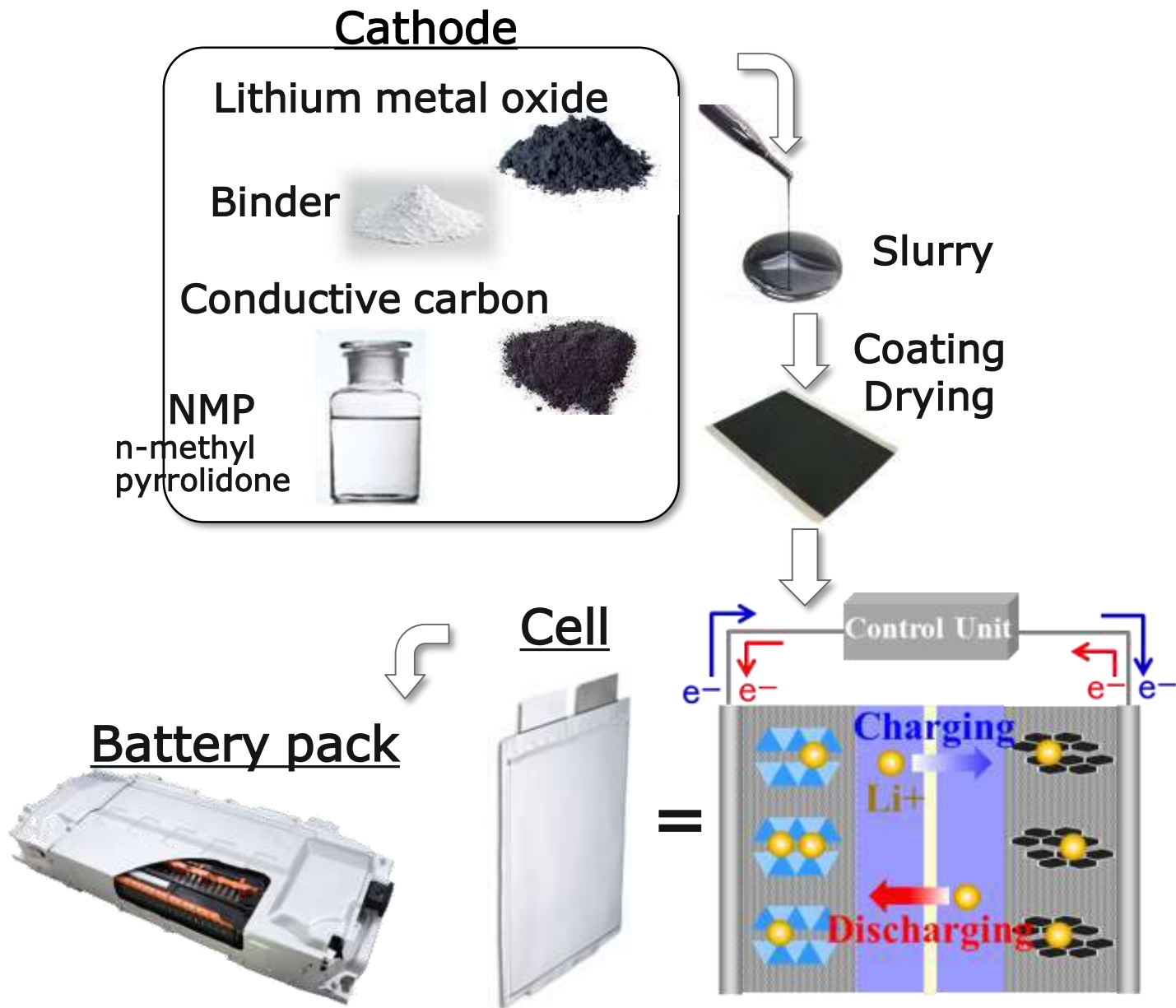
e.g. Inks, Adhesives field

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

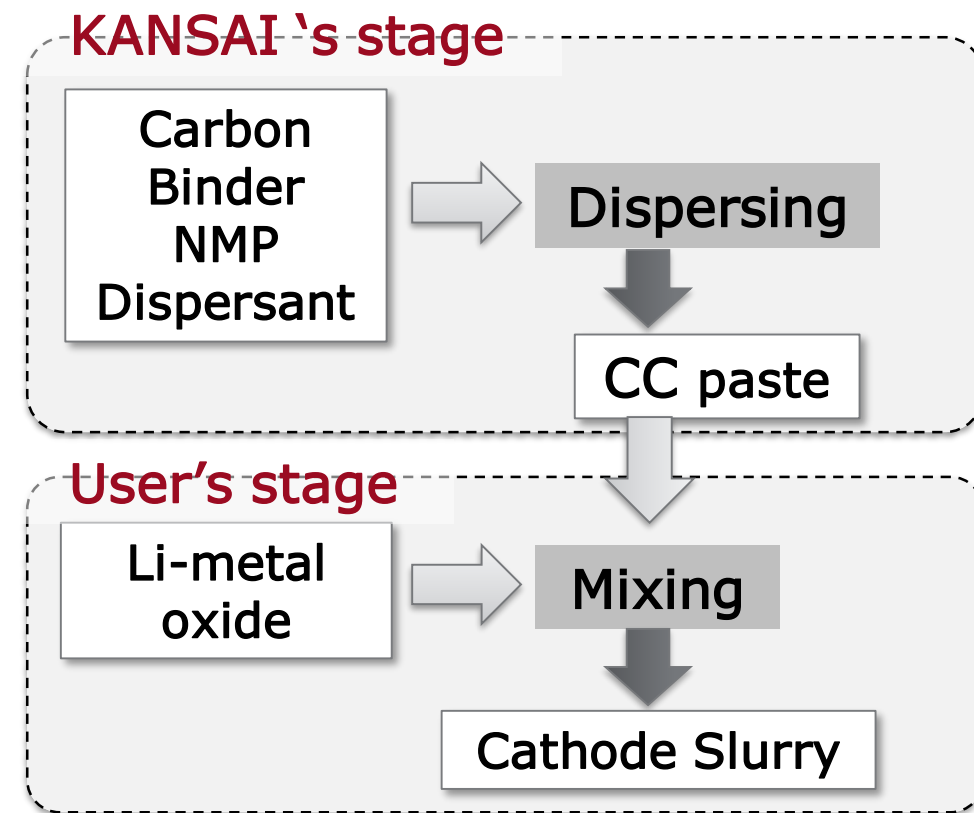


TOYOTA Yaris HV

LIB cathode manufacturing process



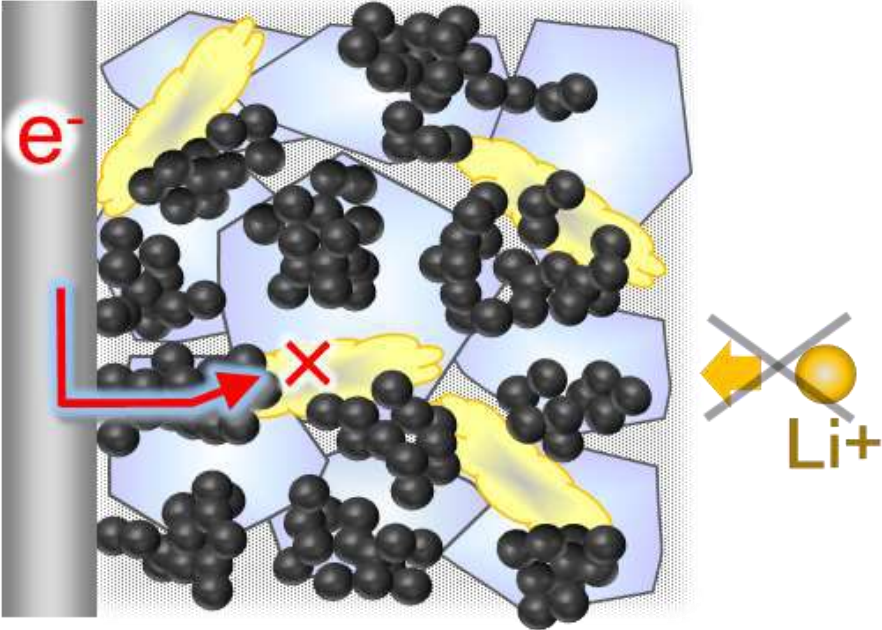
Cathode manufacturing process



CC paste : Conductive carbon paste

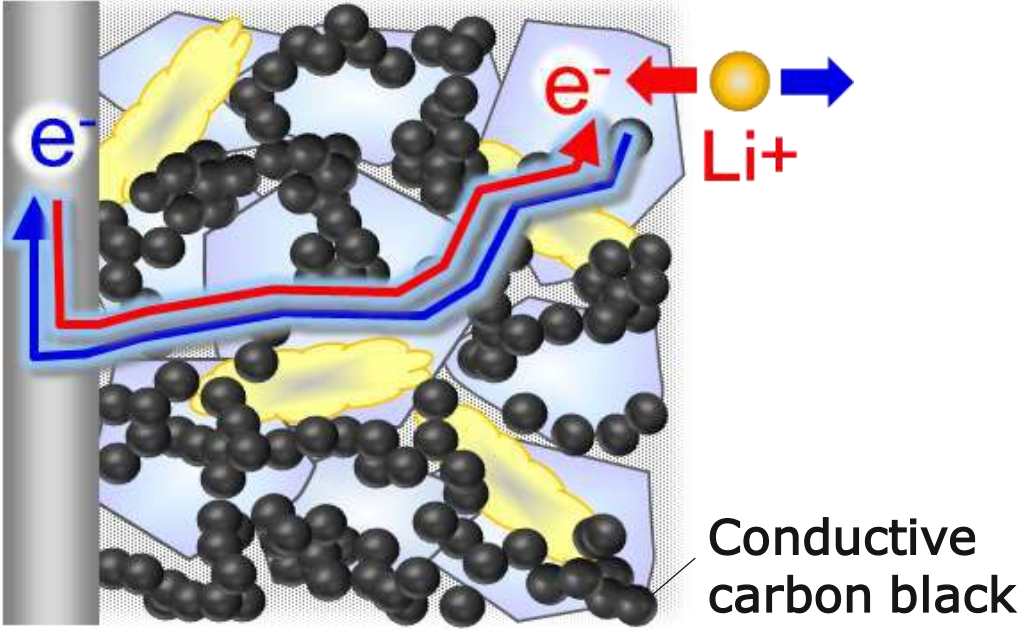
Ideal dispersing state for conductive carbon black

Insufficient dispersing



Carbon aggregated
= **hard** for electron to move

Ideal dispersing

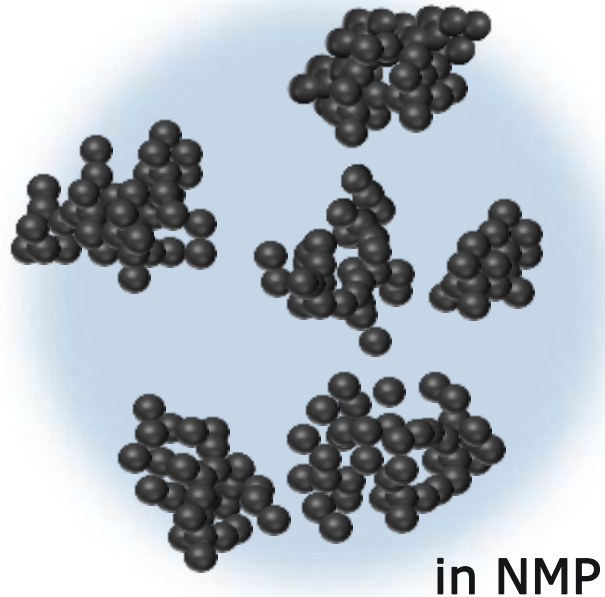


Carbon chained
= **easy** for electron to move

Problems of CC paste with insufficient dispersing

CC paste : Conductive carbon paste

Insufficient dispersing

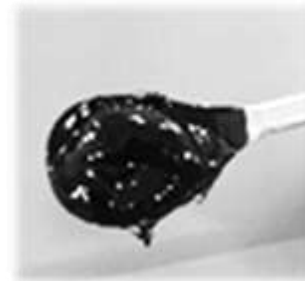


1. Carbon caking in CC paste
2. Thickening of CC paste
3. Filtration trouble of CC paste
4. Defects on cathode film
5. Poor battery performance

Caking



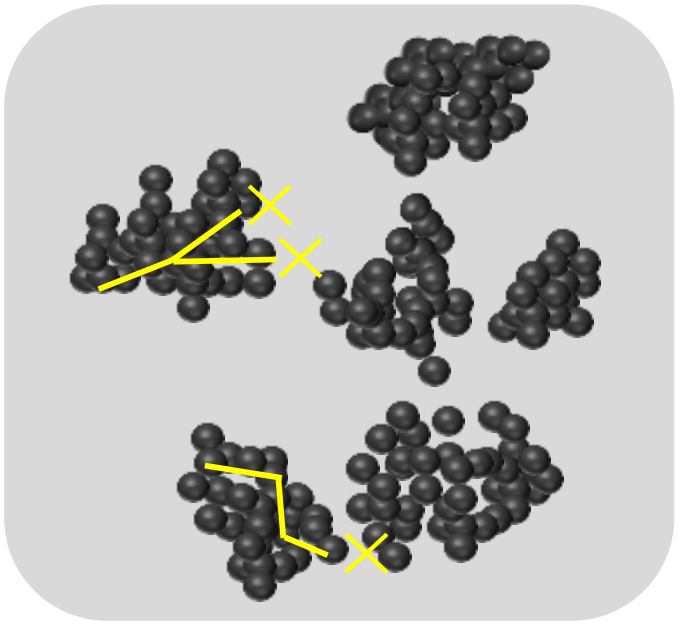
Thickening



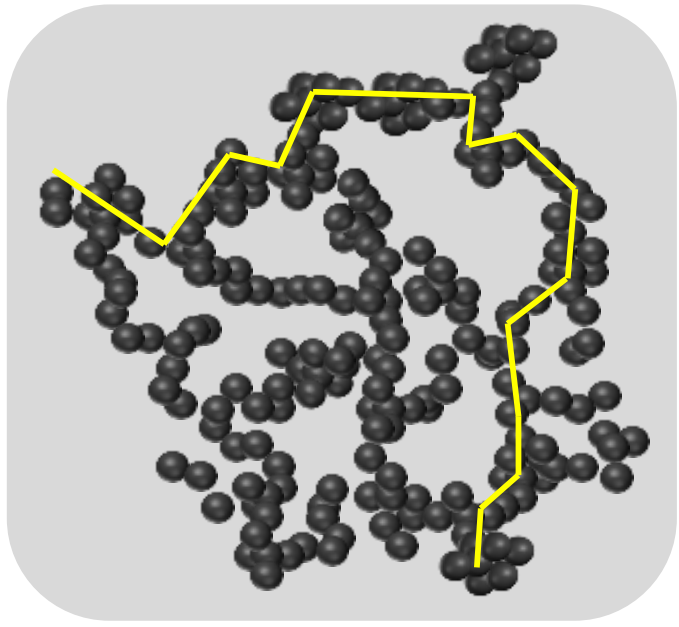
Film defect (e.g. hole)



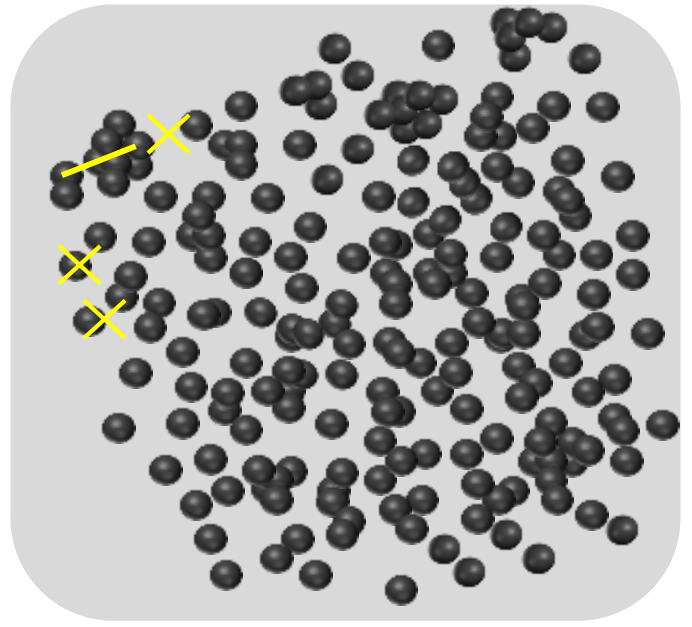
Insufficient dispersing



Ideal dispersing



Excess dispersing



Good battery performance



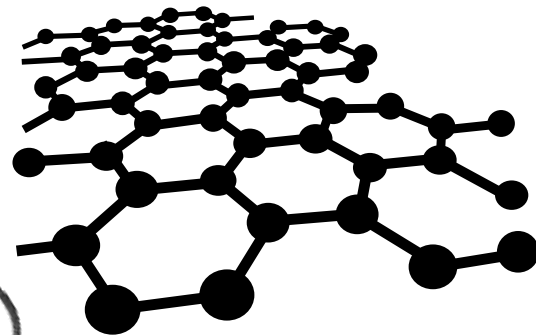
- 
- An abstract, grayscale image showing thick, flowing, brush-like strokes of varying shades of gray, creating a sense of movement and texture. The strokes are layered and overlap, with some appearing more saturated than others.
- Design of high-performance dispersants
 - Optimization dispersing process

Affinity of functional groups for graphite

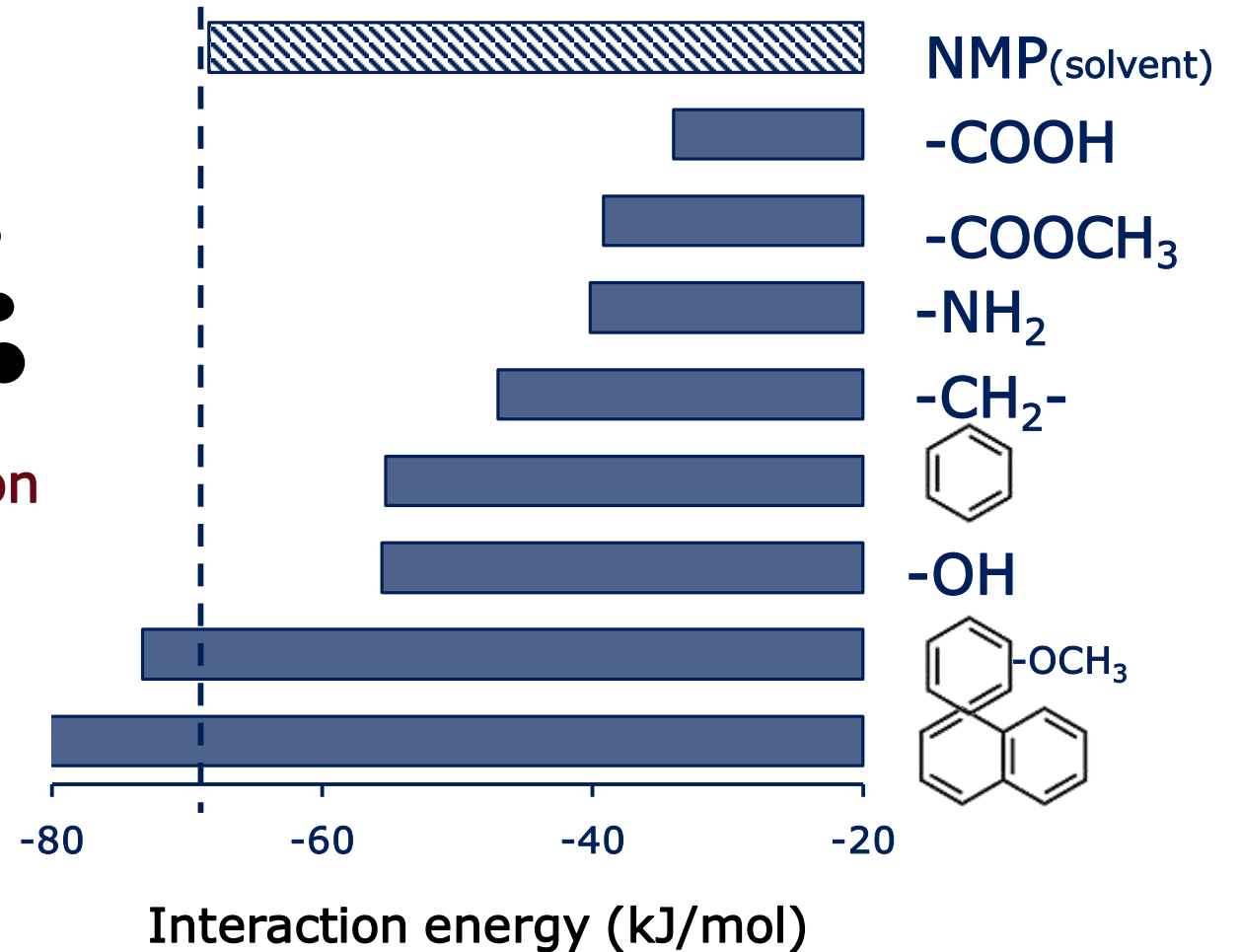
Interaction energy of functional groups onto graphite

Conductive carbon surface

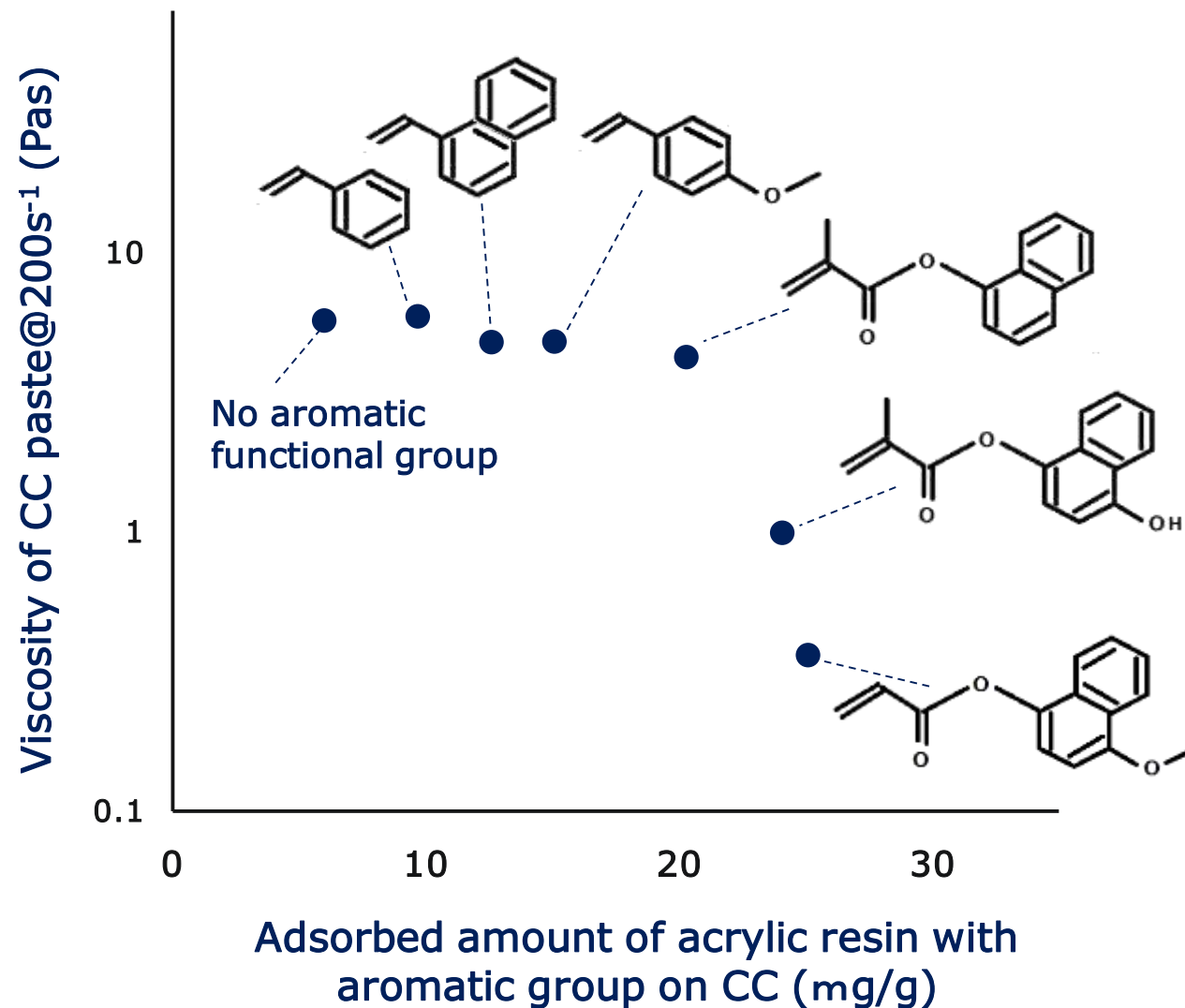
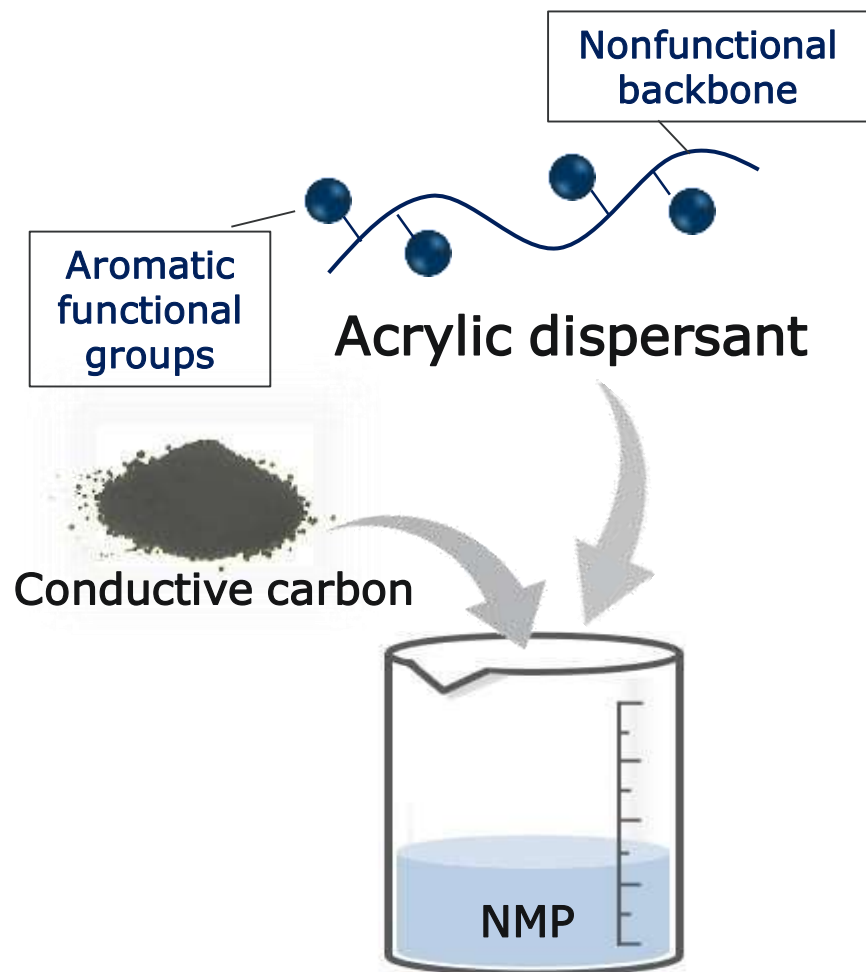
- Less oxidative site
- Graphite structure
- Hydrophobic flat plane



π - π interaction



Dispersant with aroma-ring and CC paste viscosity



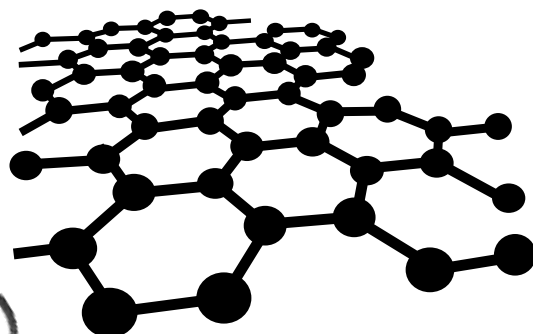
CC : Conductive carbon

Affinity of functional groups for graphite

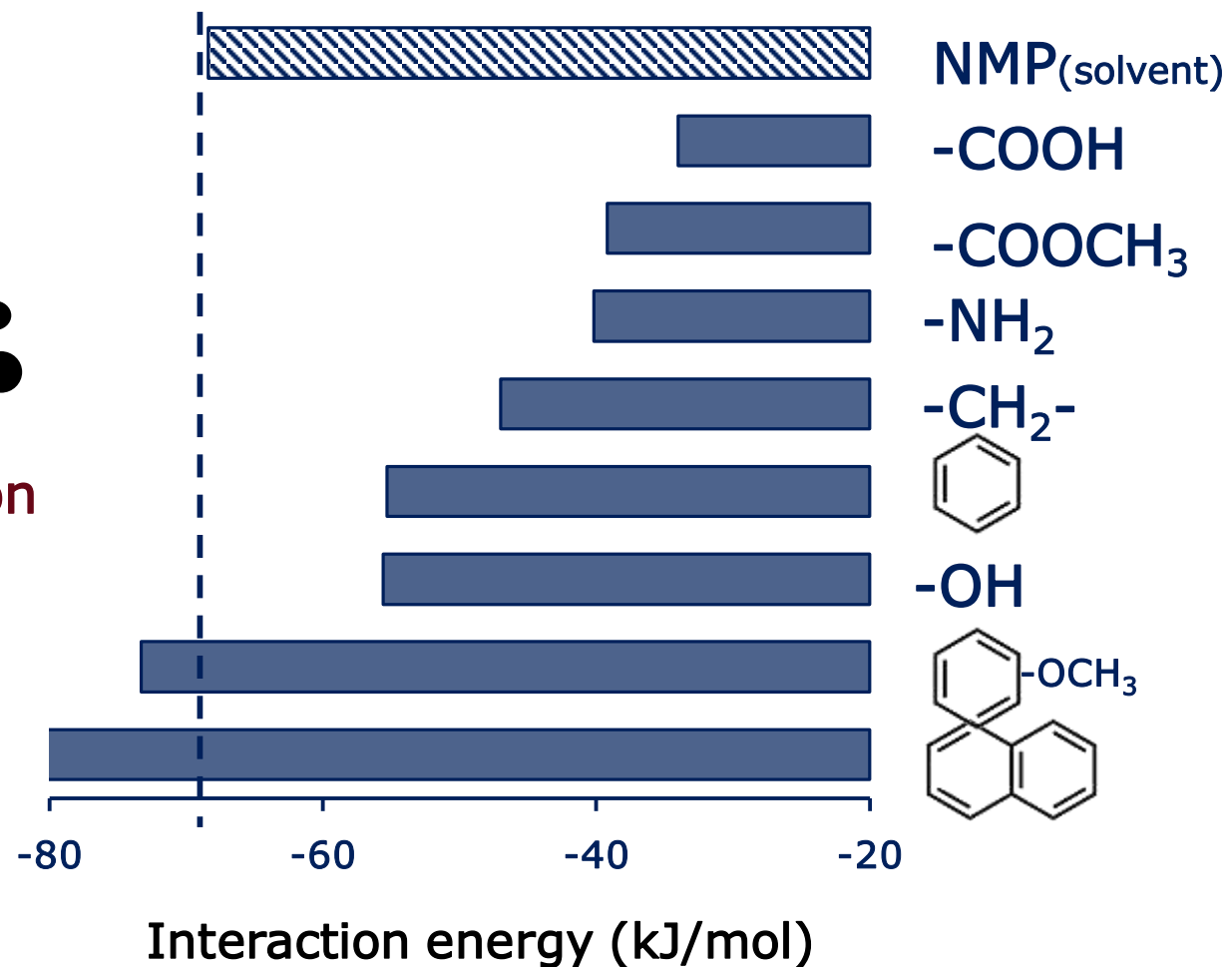
Interaction energy of functional groups onto graphite

Conductive carbon surface

- Less oxidative site
- Graphite structure
- Hydrophobic flat plane

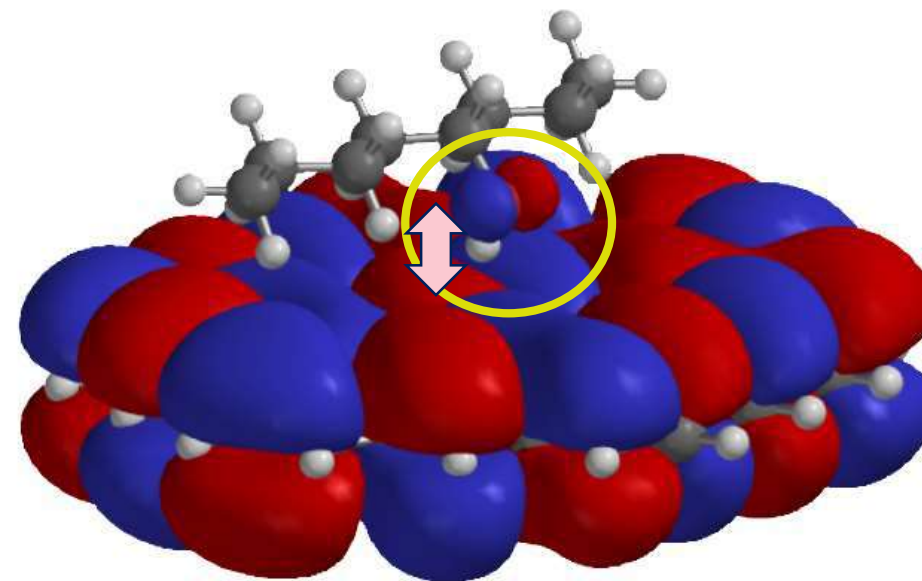
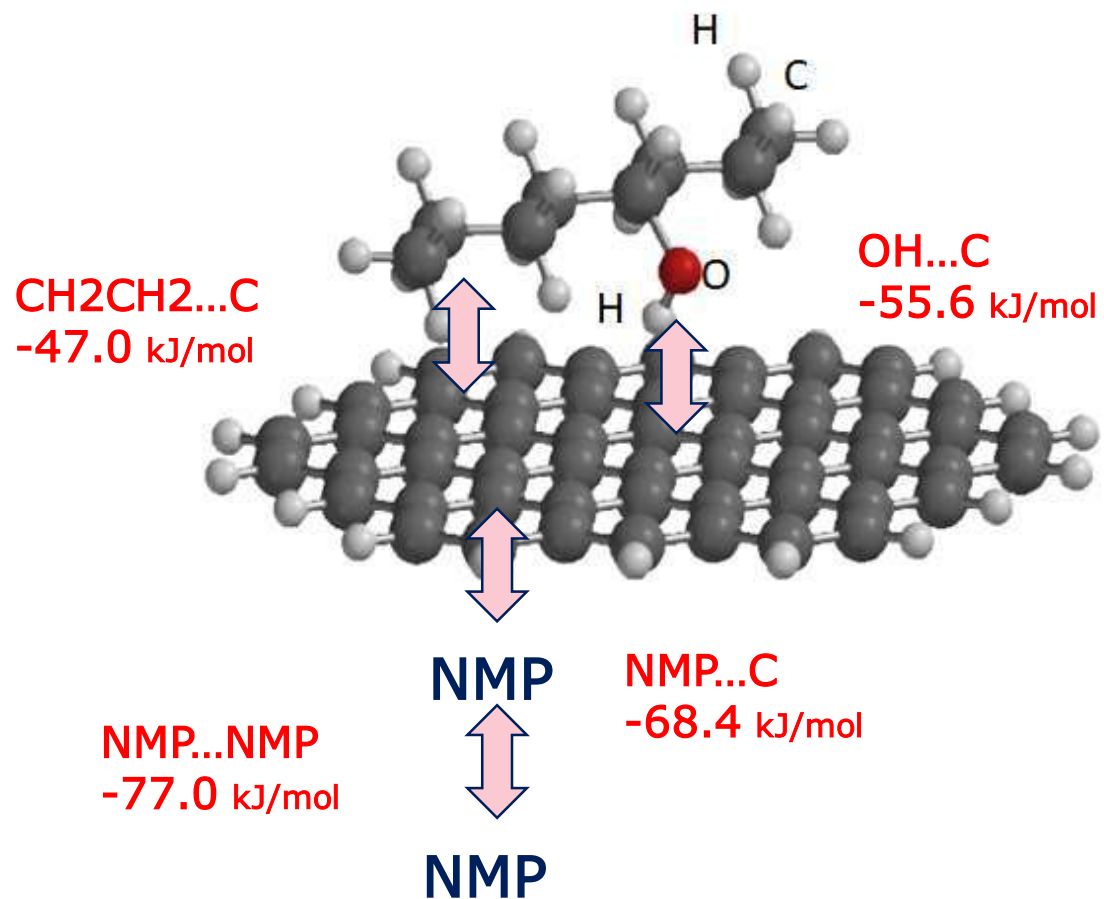


π - π interaction



Interaction energy of OH and graphite surface

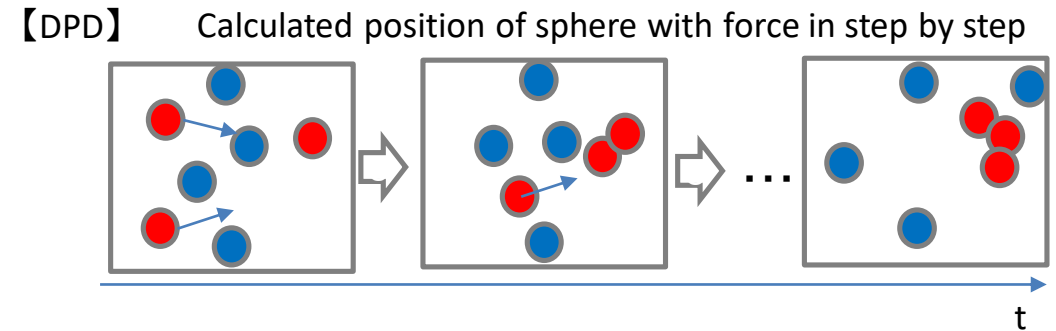
calculation basis set : ω B97X-D/6-31G(d)



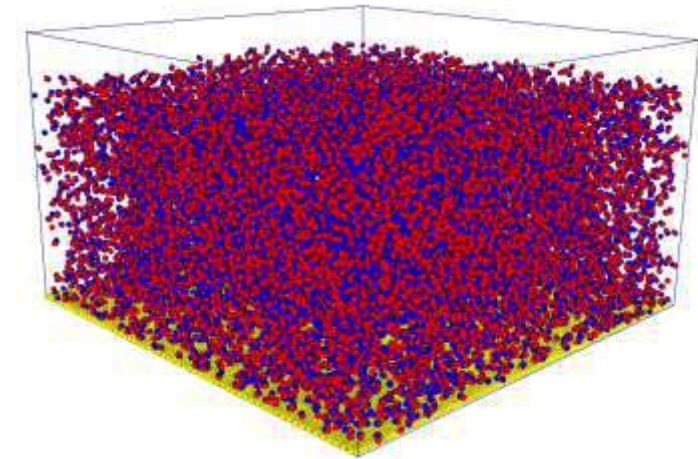
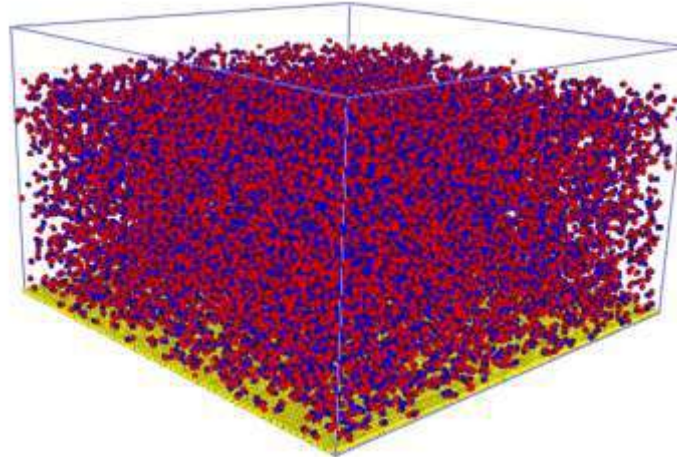
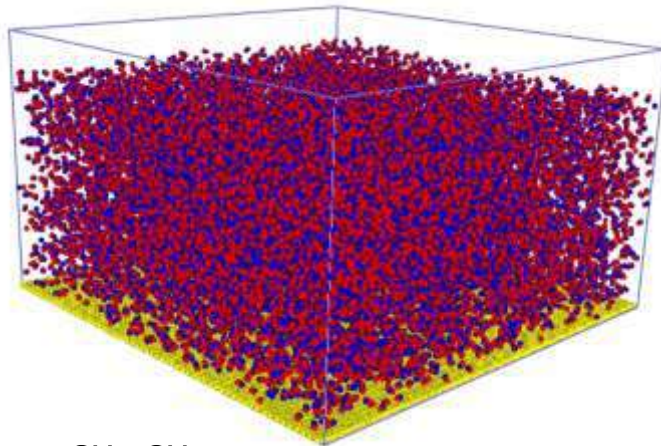
OH orbital interacted to pi orbital on graphite surface

DPD calculation of Ethanol's state in NMP on graphite

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



Initial time progression (Calculation steps)



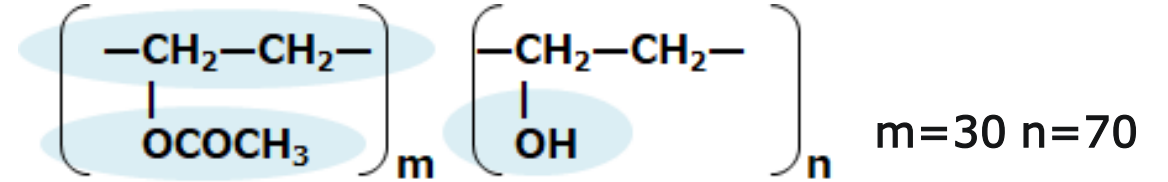
Blue : -CH₂-CH₂-
Red : -OH
NMP : not displayed

<http://octa.com>

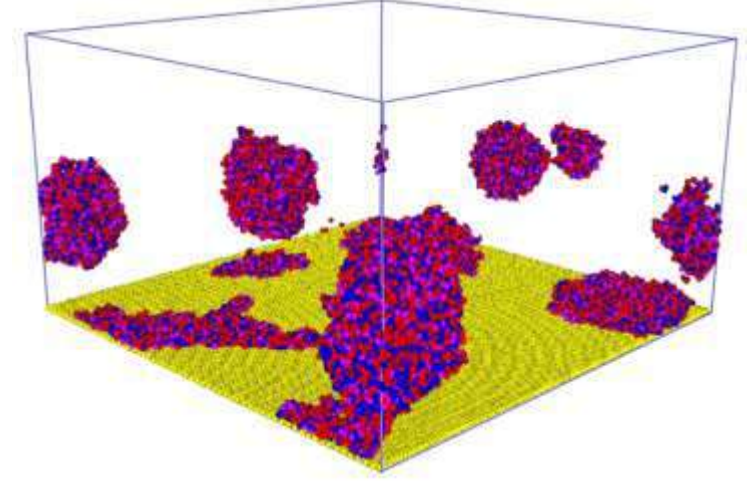
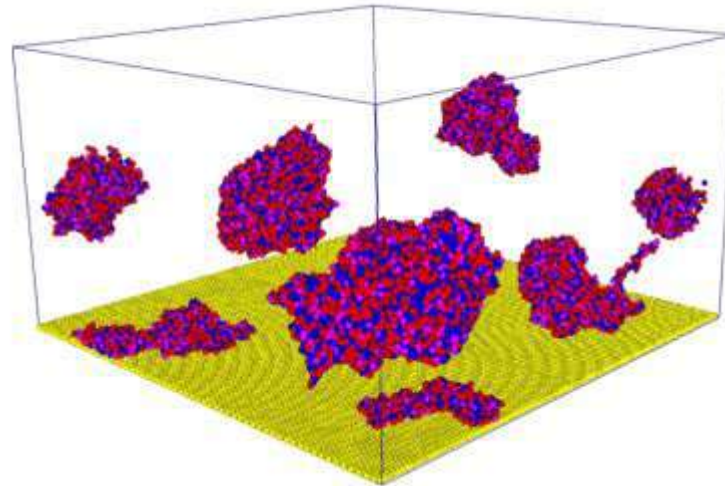
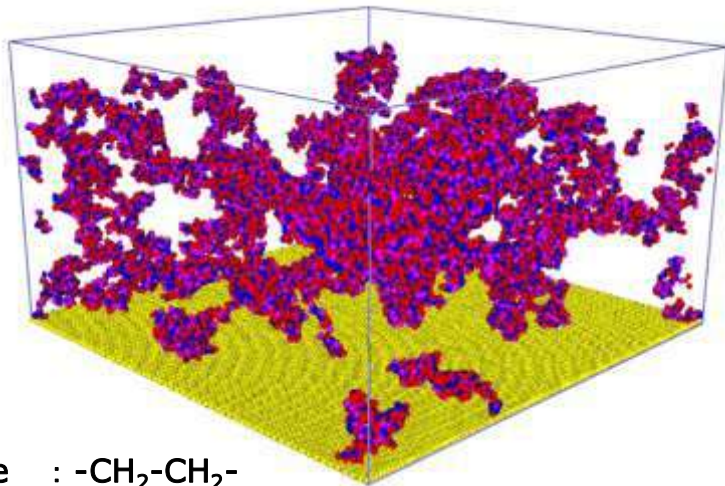
Ethanol : adsorption onto graphite < thermal diffusion into NMP

DPD calculation of PVA's state in NMP on graphite

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



Initial time progression (Calculation steps) ➔



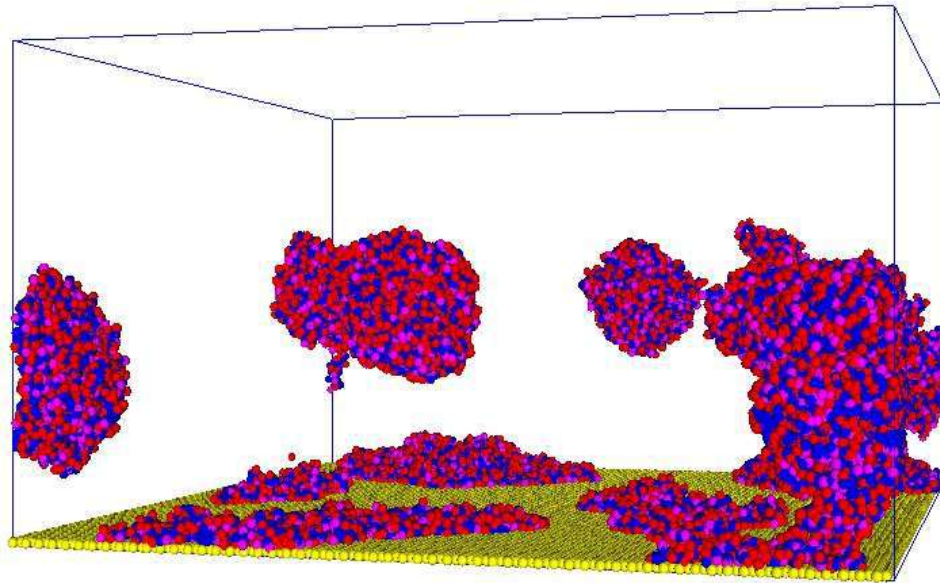
Blue : -CH₂-CH₂-
Red : -OH
Purple : -OCOCH₃
NMP : not displayed

<http://octa.com>

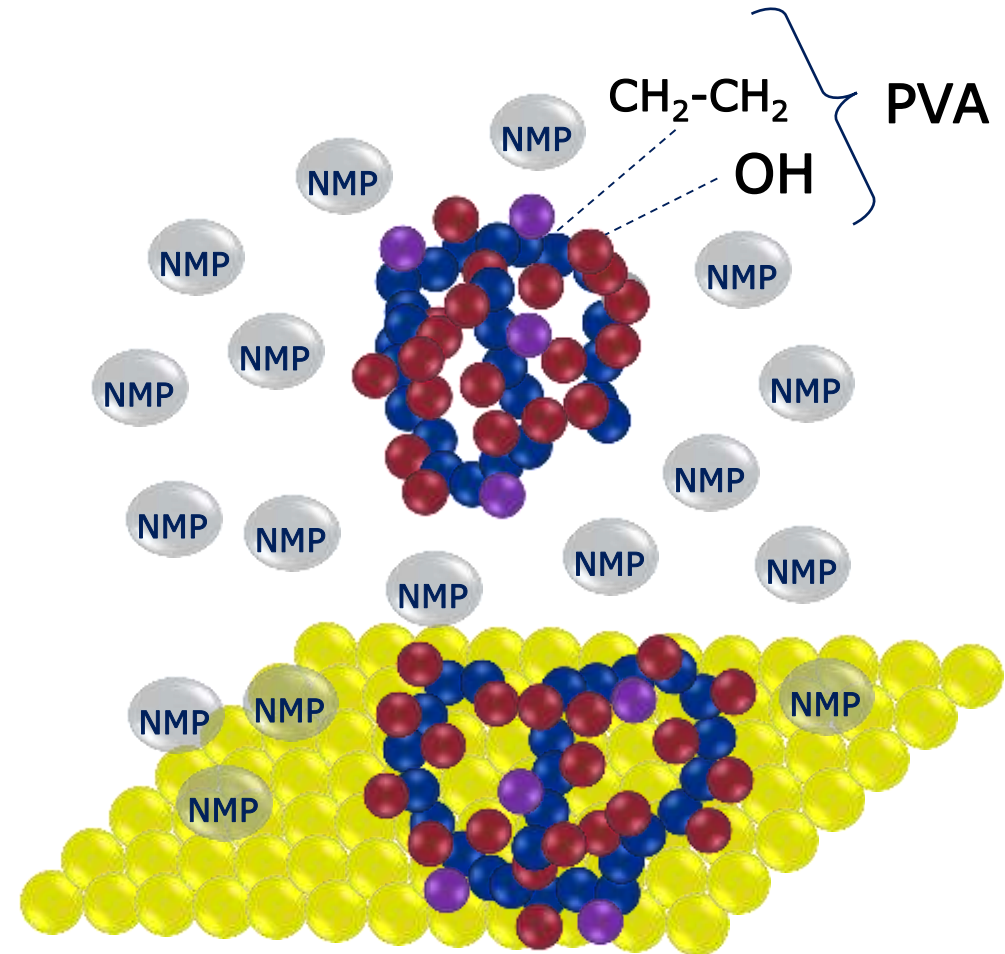
PVA polymer : adsorption onto graphite > thermal diffusion into NMP

DPD calculation of PVA's state in NMP on graphite

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

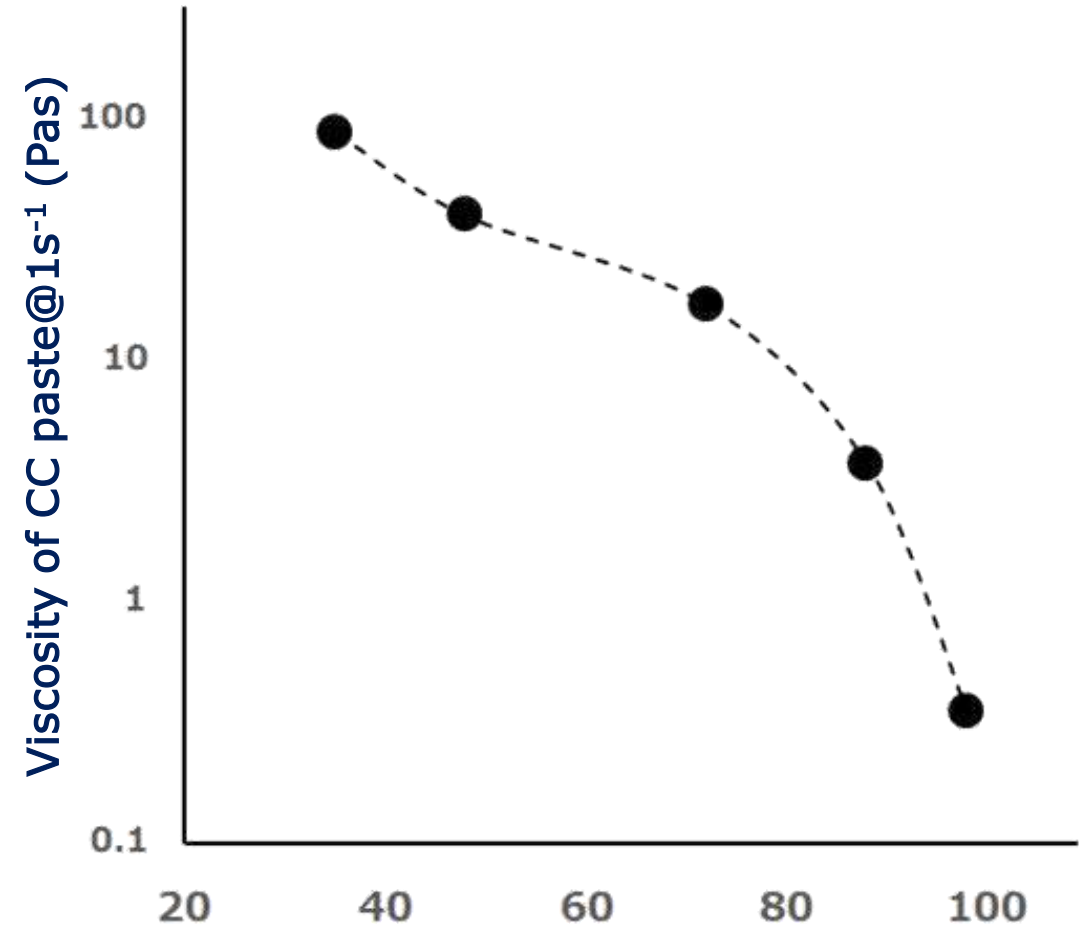
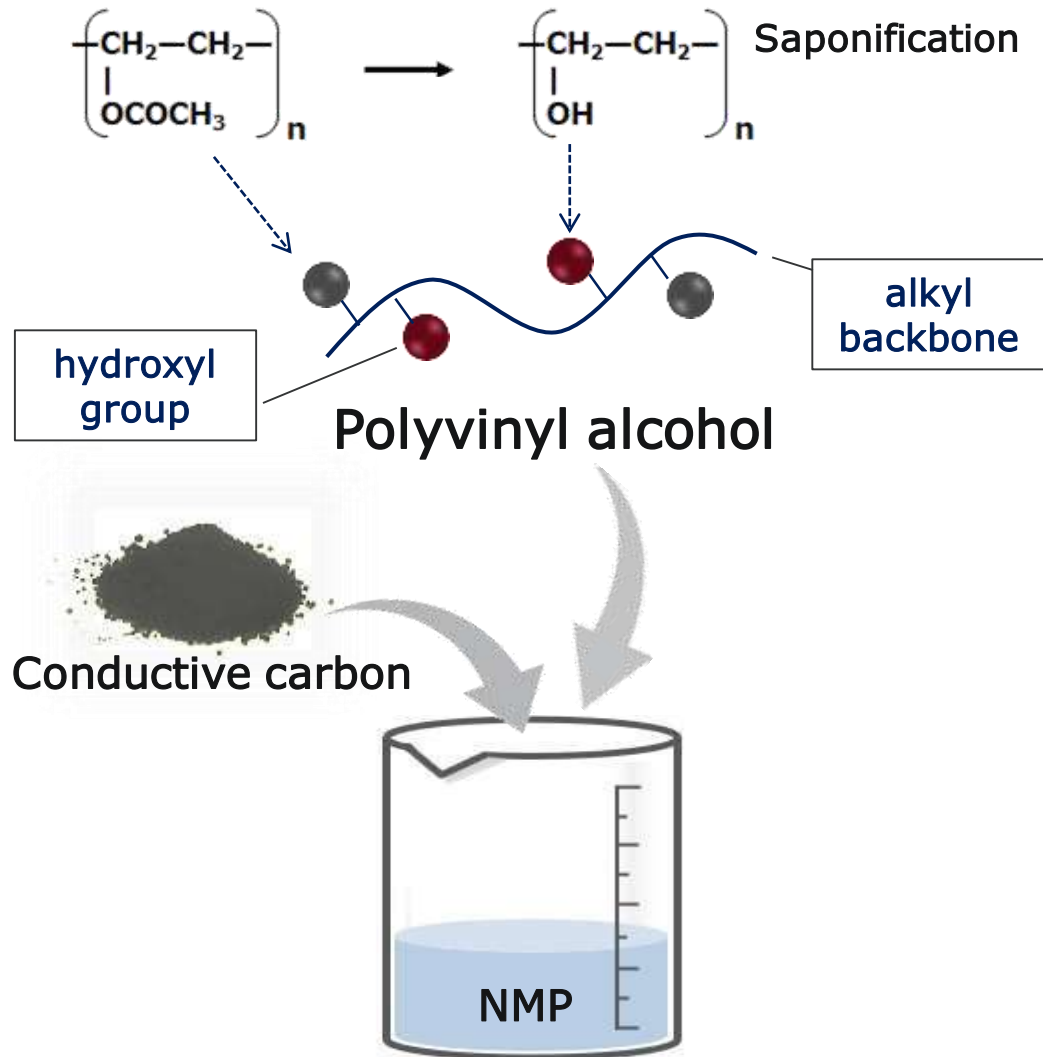


NMP: not displayed



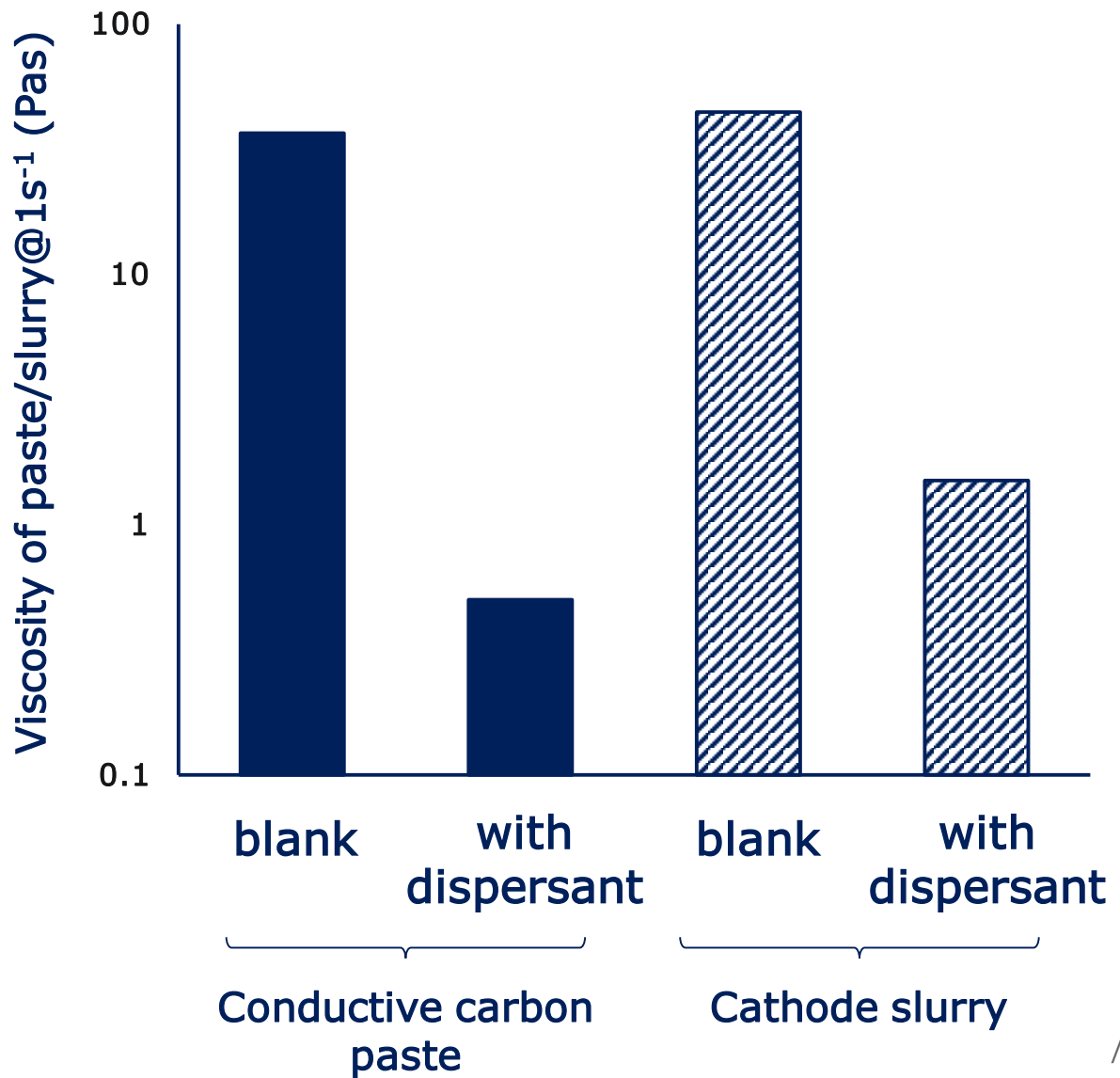
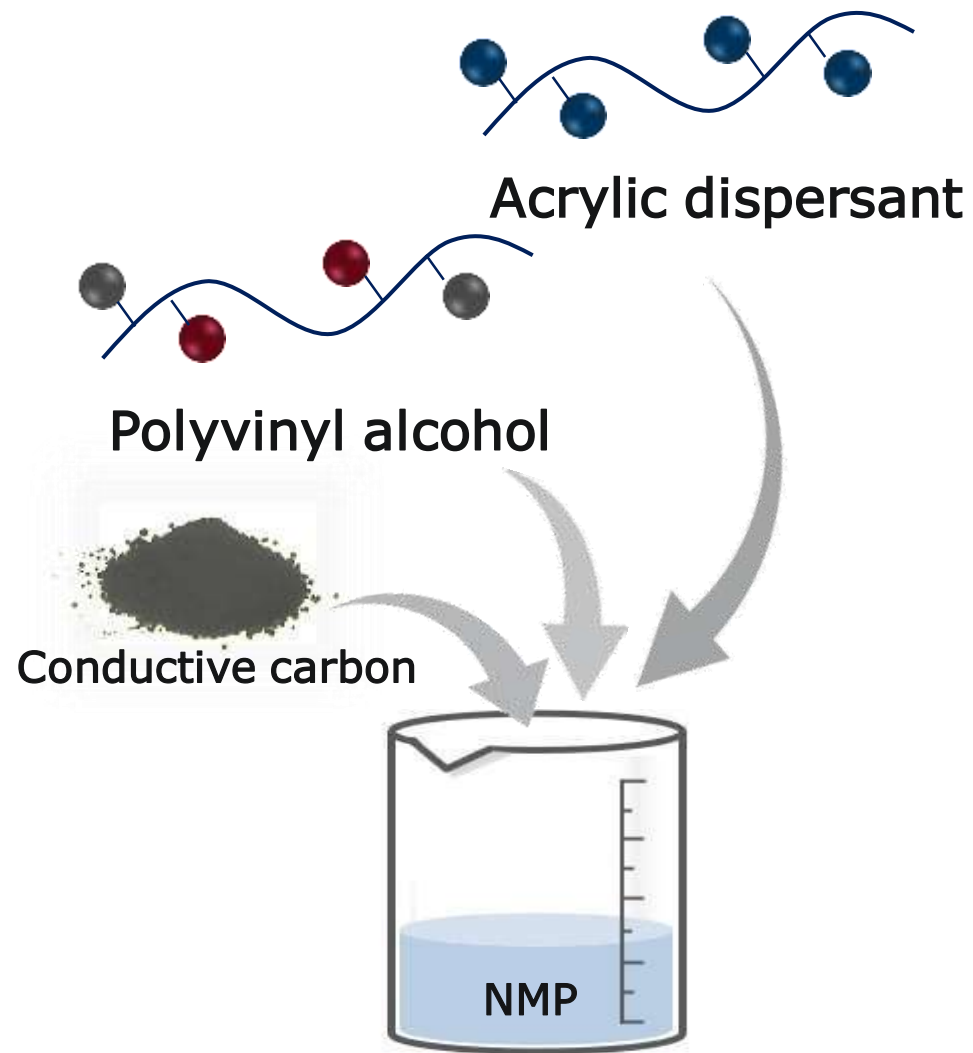
Graphite
Conductive carbon surface

Dispersant with -OH and CC paste viscosity

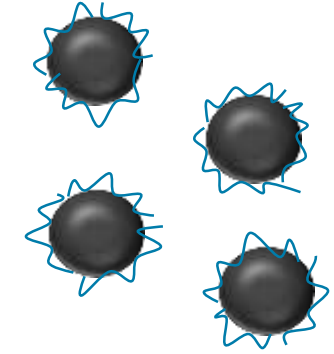
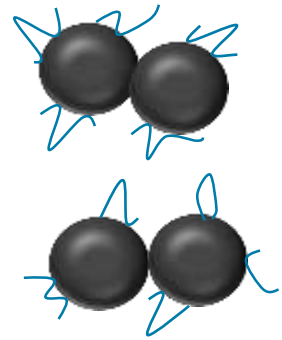
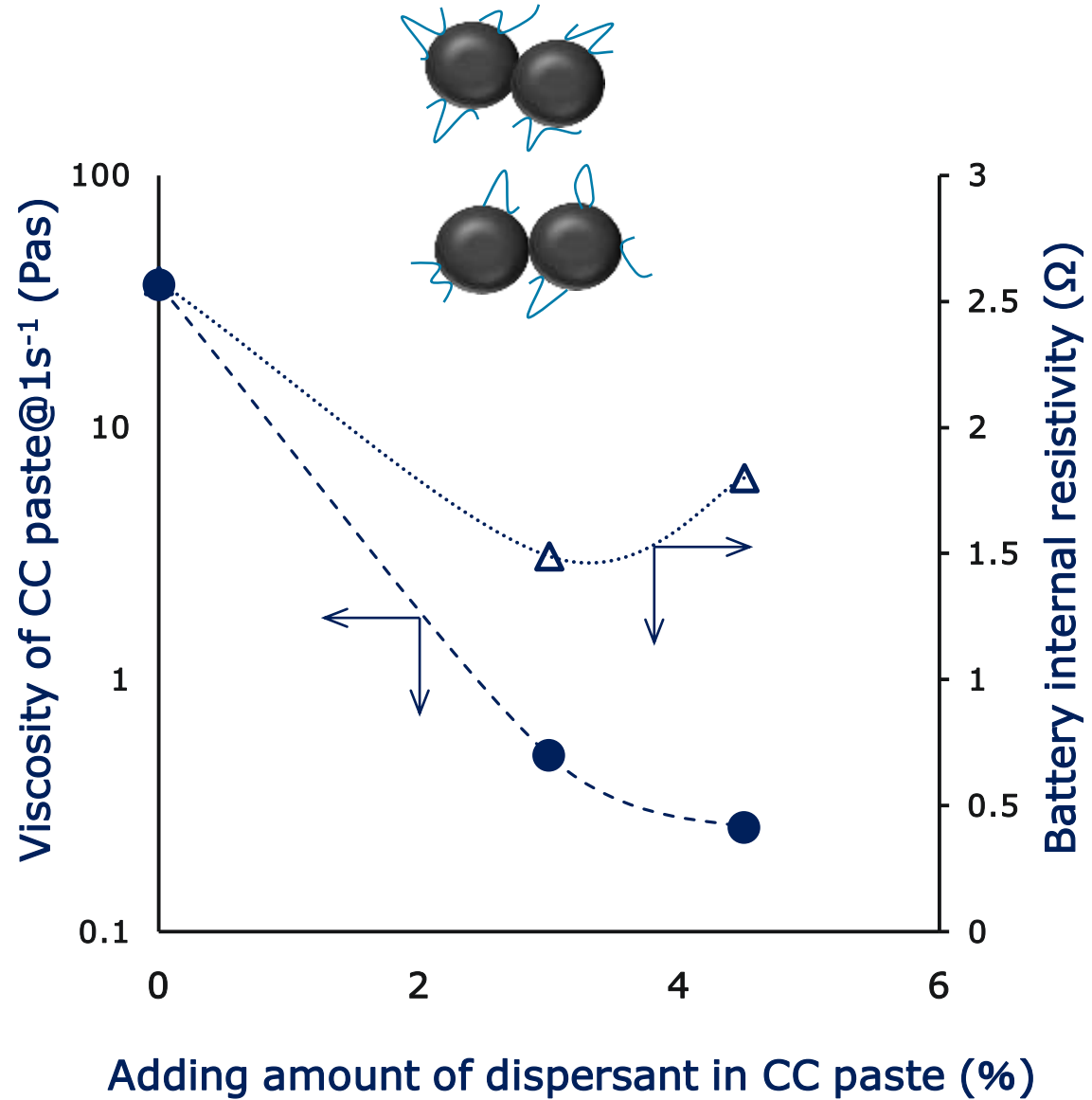
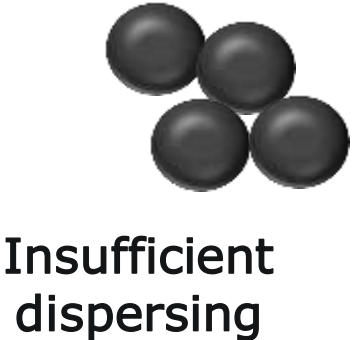


Saponification value of PVA(%)
 : hydroxyl group content

Combination of suitable dispersant and paste viscosity



Amount of dispersant in CC paste and performance

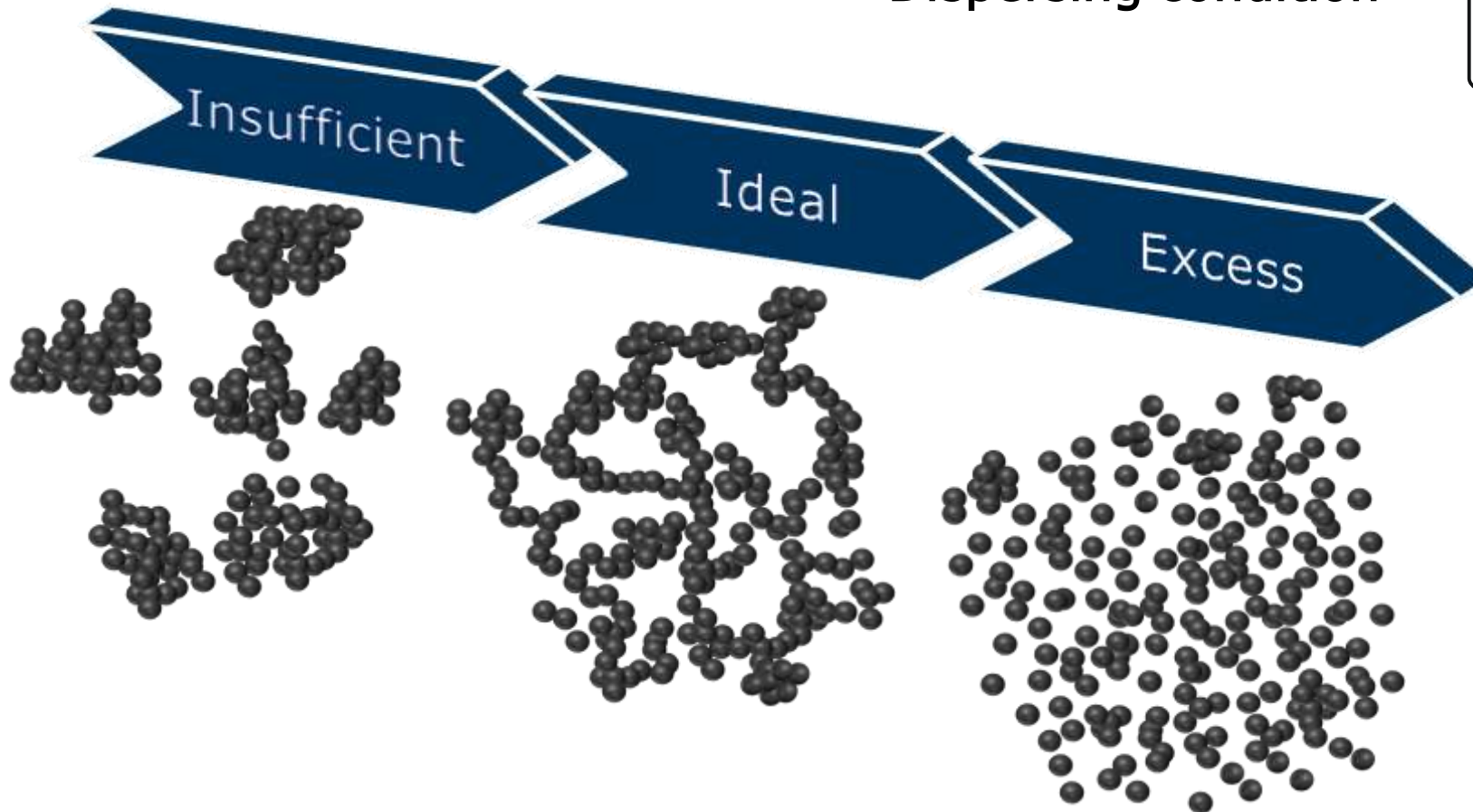
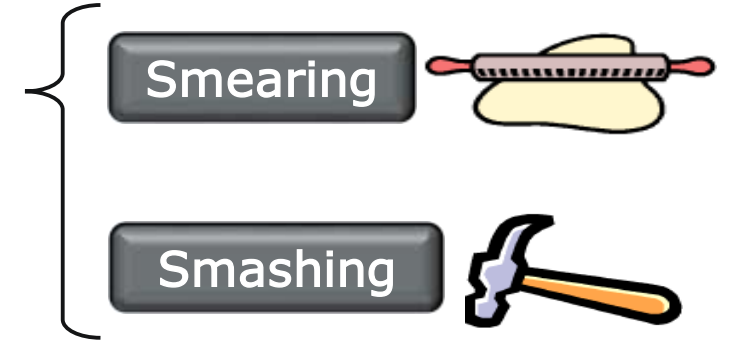


- Over dispersing
- Excessive addition of insulating dispersant

Optimization of dispersion process

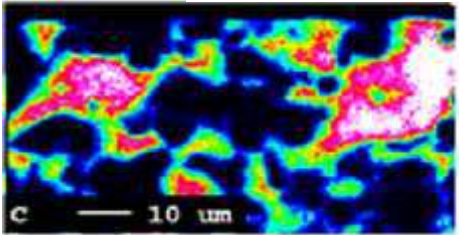
Adjustment in degree of carbon dispersion

- Dispersing system
- Dispersing apparatus
- Dispersing condition

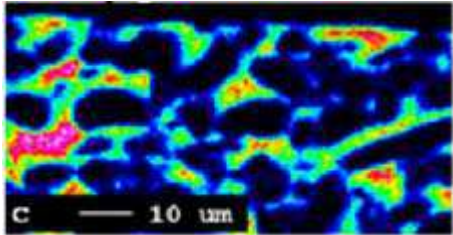
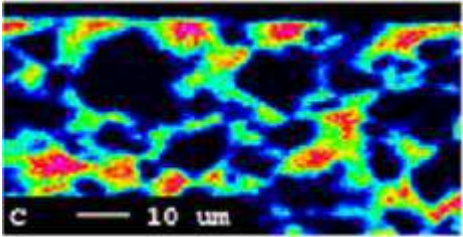


Dispersion progression of CC paste and performance

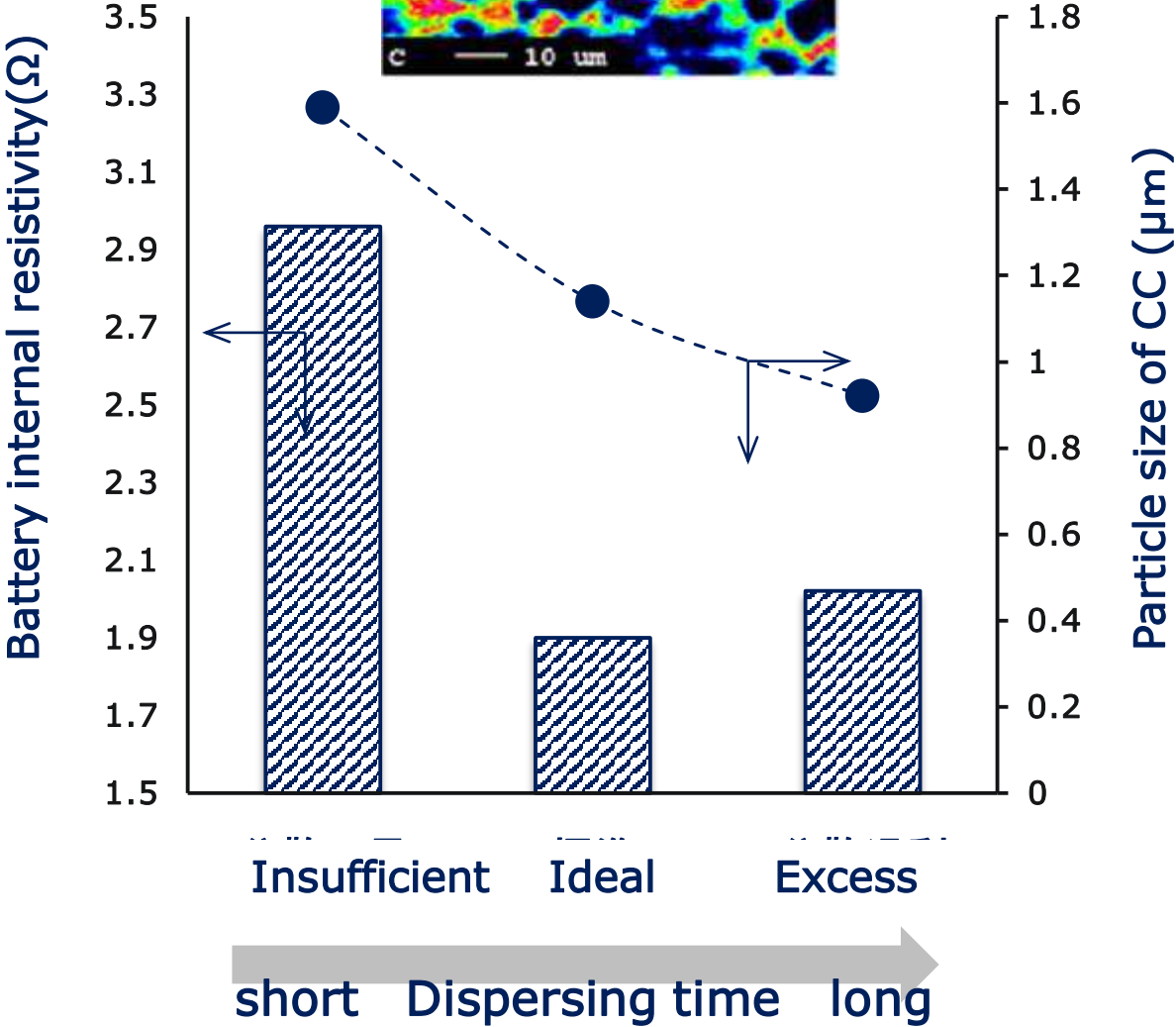
Cross-section image of cathode
EPMA C element mapping



Carbon agglomeration
Disconnection of conductive paths



Carbon isolation
Disconnection of conductive paths

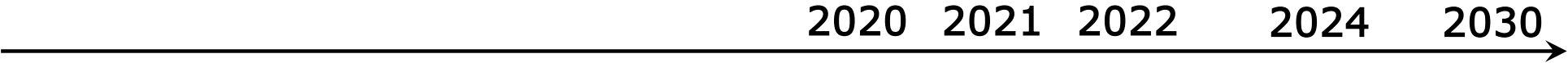


A large, abstract graphic on the left side of the slide, consisting of thick, overlapping brushstrokes in shades of grey and white, creating a sense of motion and texture.

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



Acetylene carbon black
(in NMP)

for HEV cathode



Smaller size



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**

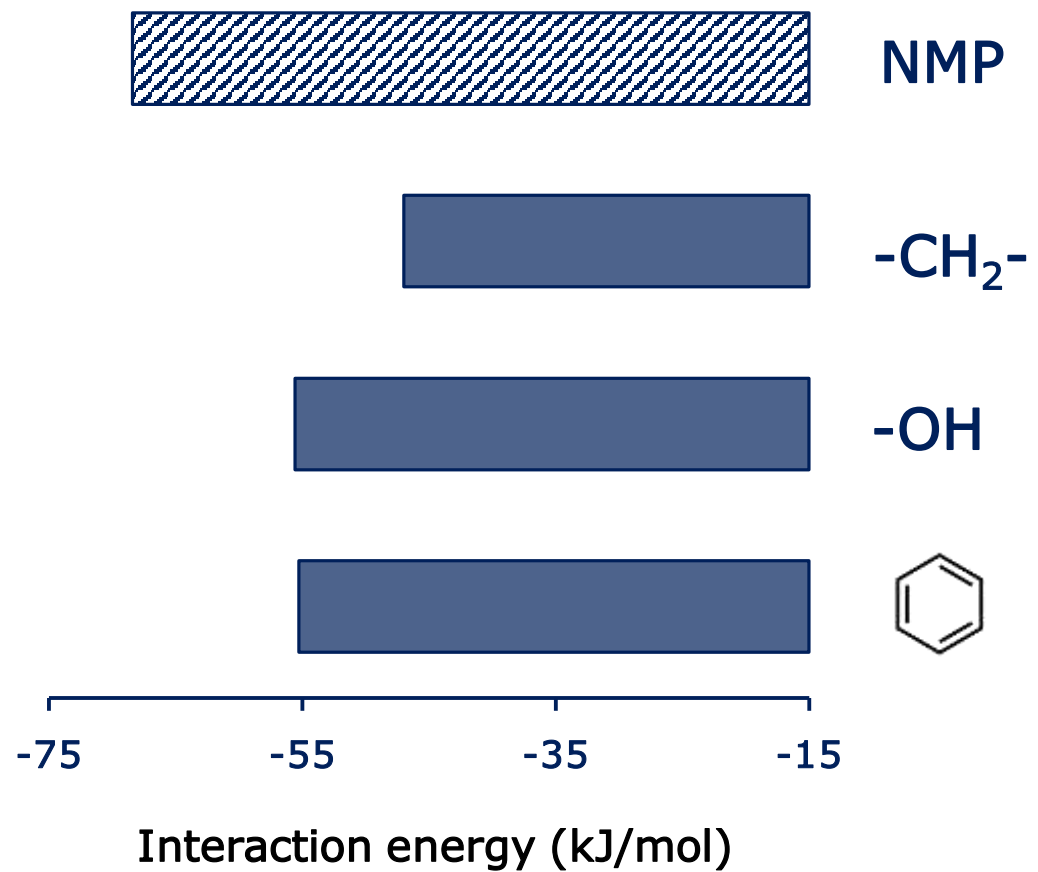


MW-CNT

Feasibility study



Affinity of functional groups vs NMP for graphite



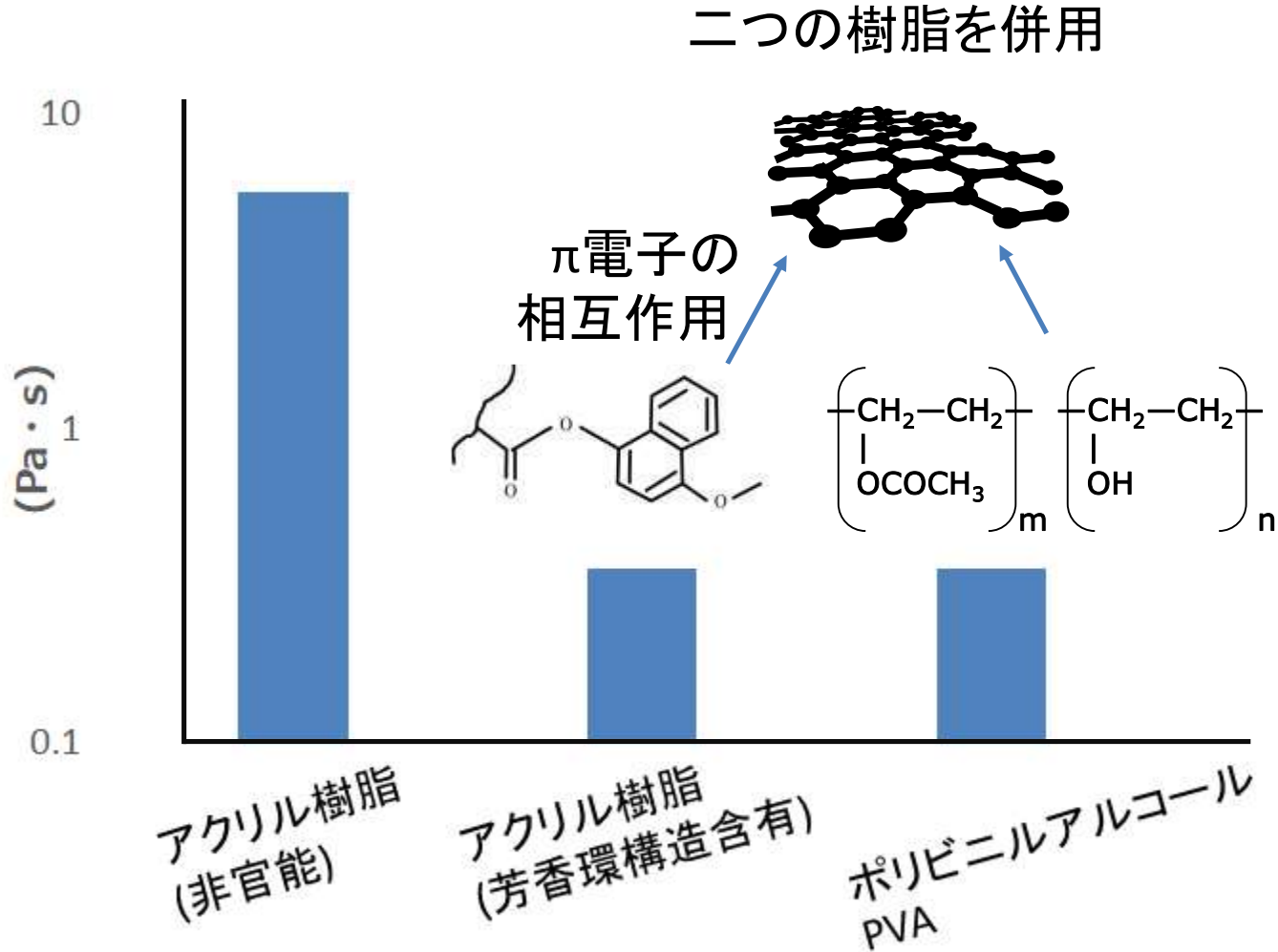
Interaction energy with carbon surface

NMP (solvent) > Phenyl = OH

1. What is a good functional group for dispersing

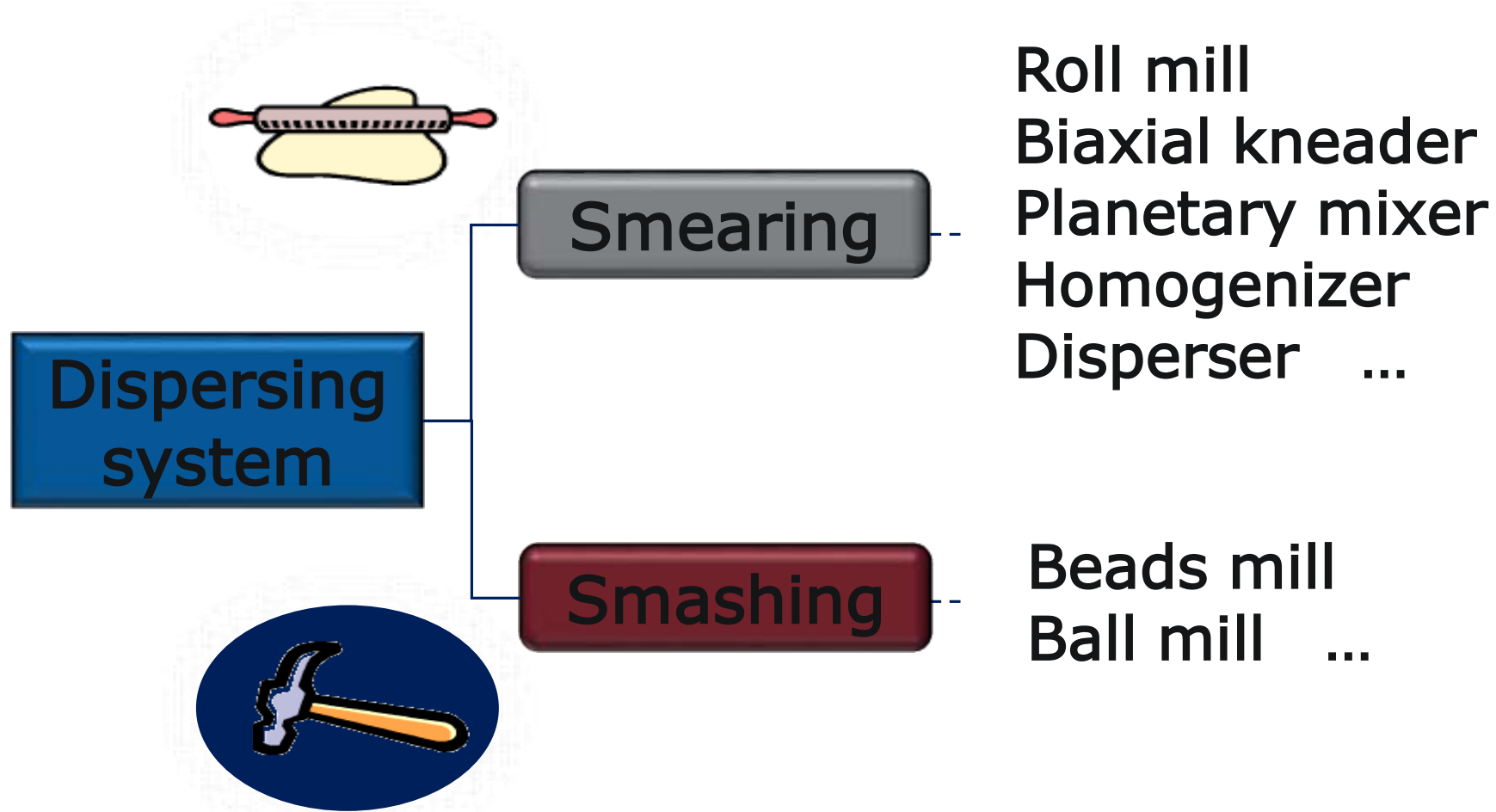
Formulation design

図3・分散剤種添加によるせん断速度
200/sにおける導電性カーボンペースト
の粘度-ペースト粘度



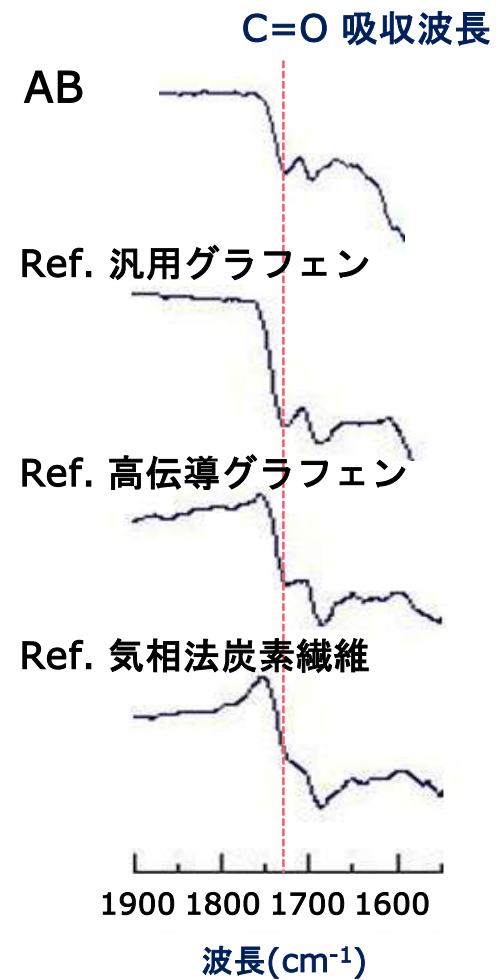
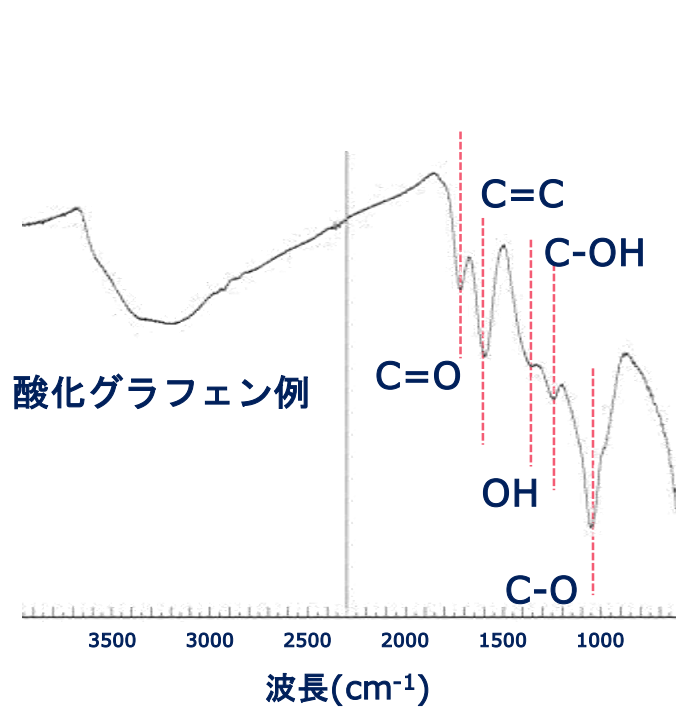
芳香環構造だけでなく、PVAも相互作用により吸着・分散効果があることがわかった。

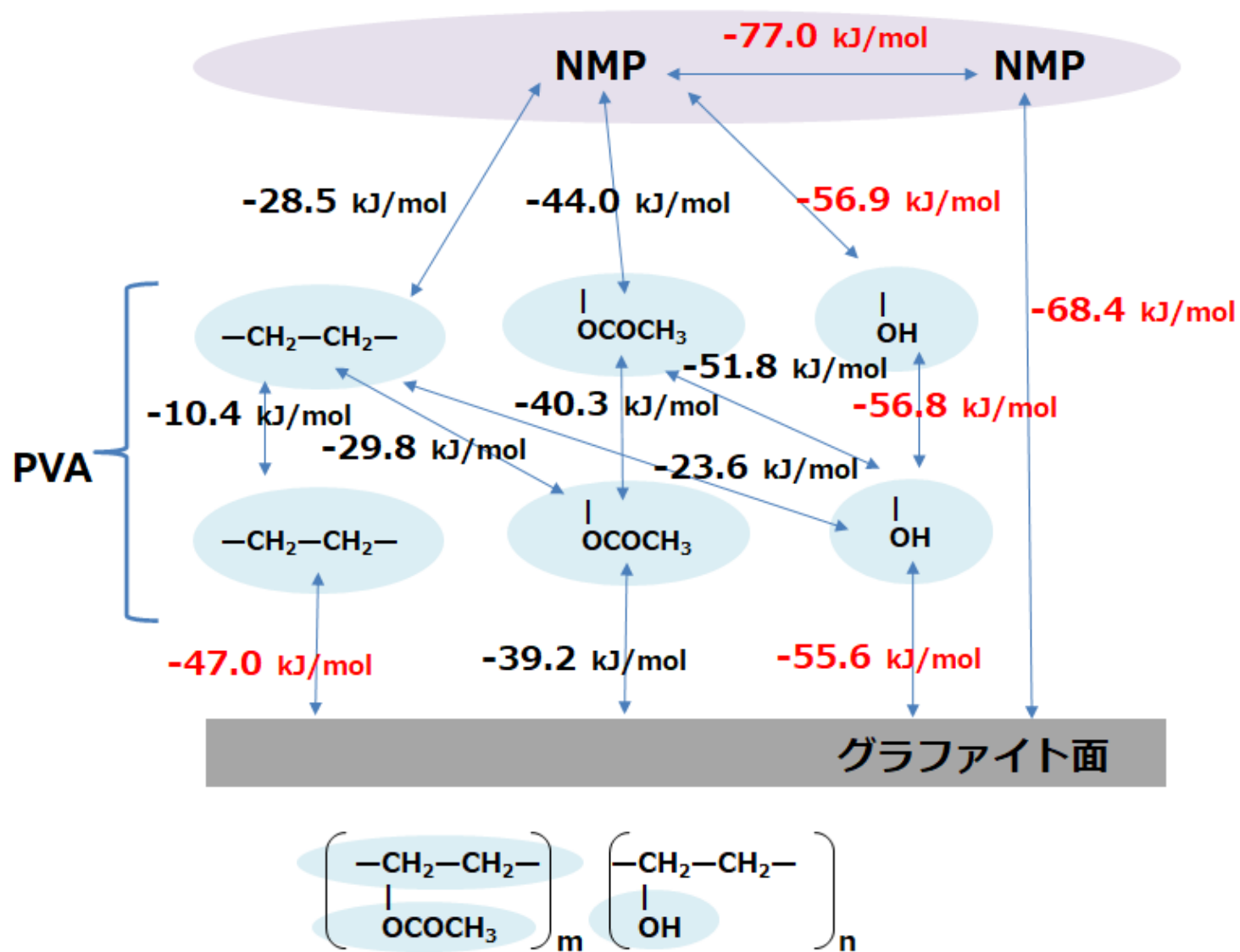
1. Optimizing the dispersing process



KANSAI has various dispersing methods

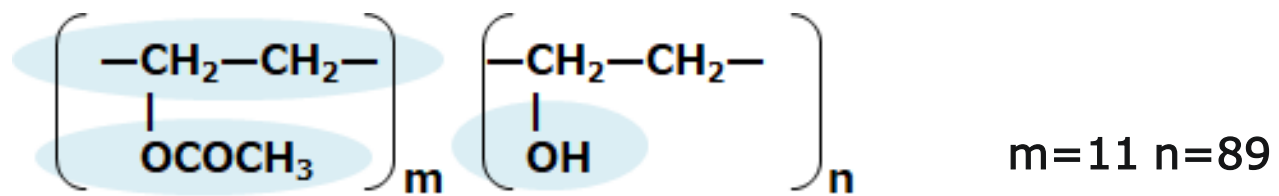
Why dose the OH group interact carbon surface?





DPDの結果

Formulation design



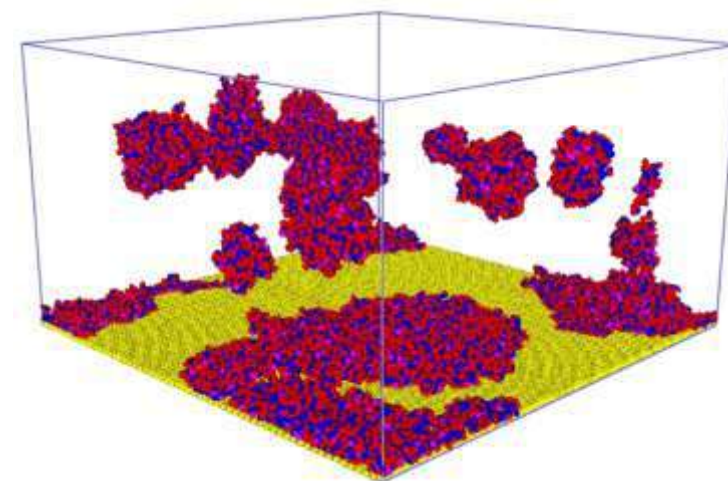
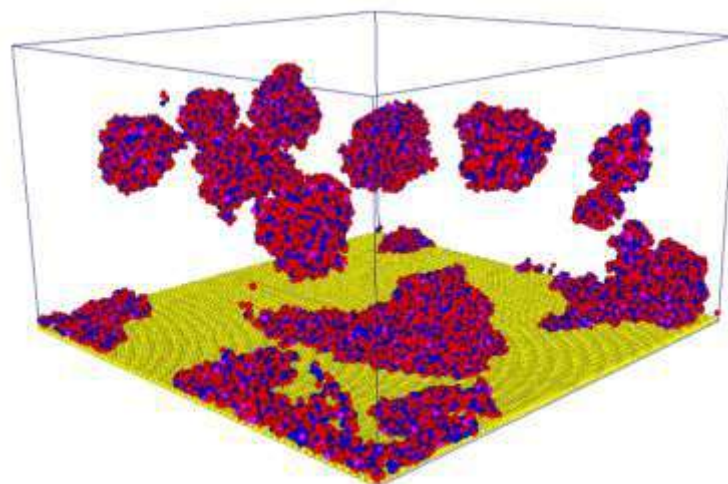
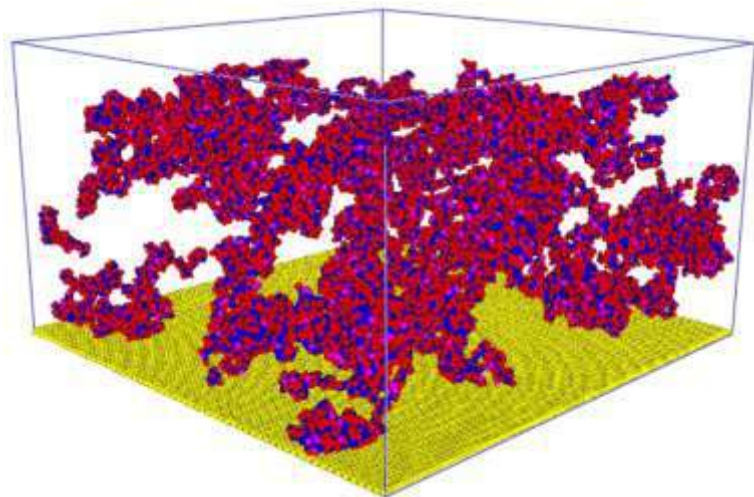
Initial



Time1

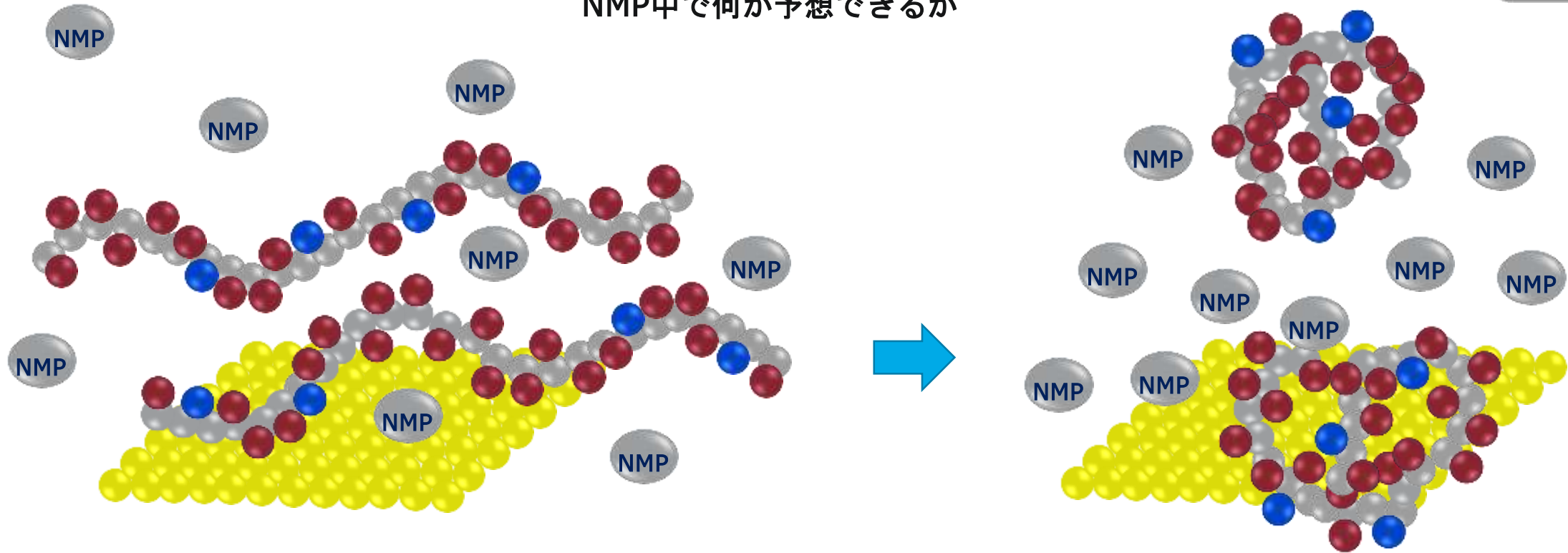


Time2



Formulation
design

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