An ALS XAS characterization and DFT calculation guided materials discovery of conductive polymer binders for high capacity Si anode electrode

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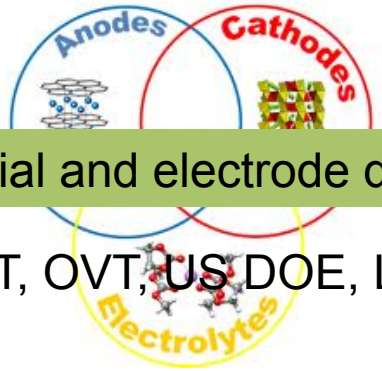
Ask not what your country can do for you - ask what you can do for your country- JFK

From Fundamental Science to Application at Lawrence Berkeley Lab

Technology development



Battery material and electrode development/testing

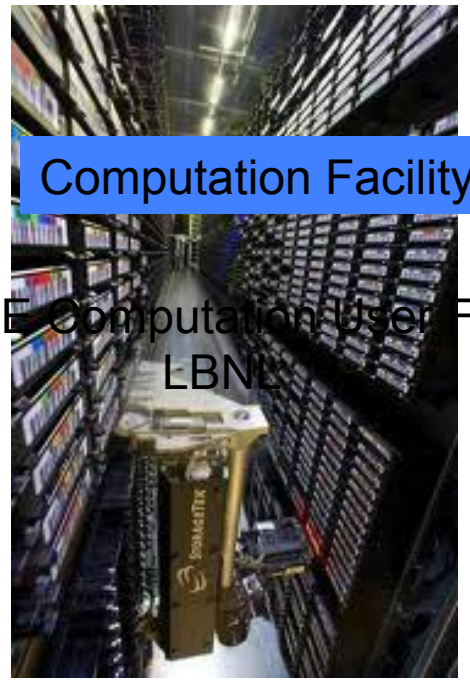
BATT, OVT, US DOE, LBNL

Basic sciences

ALS Analysis

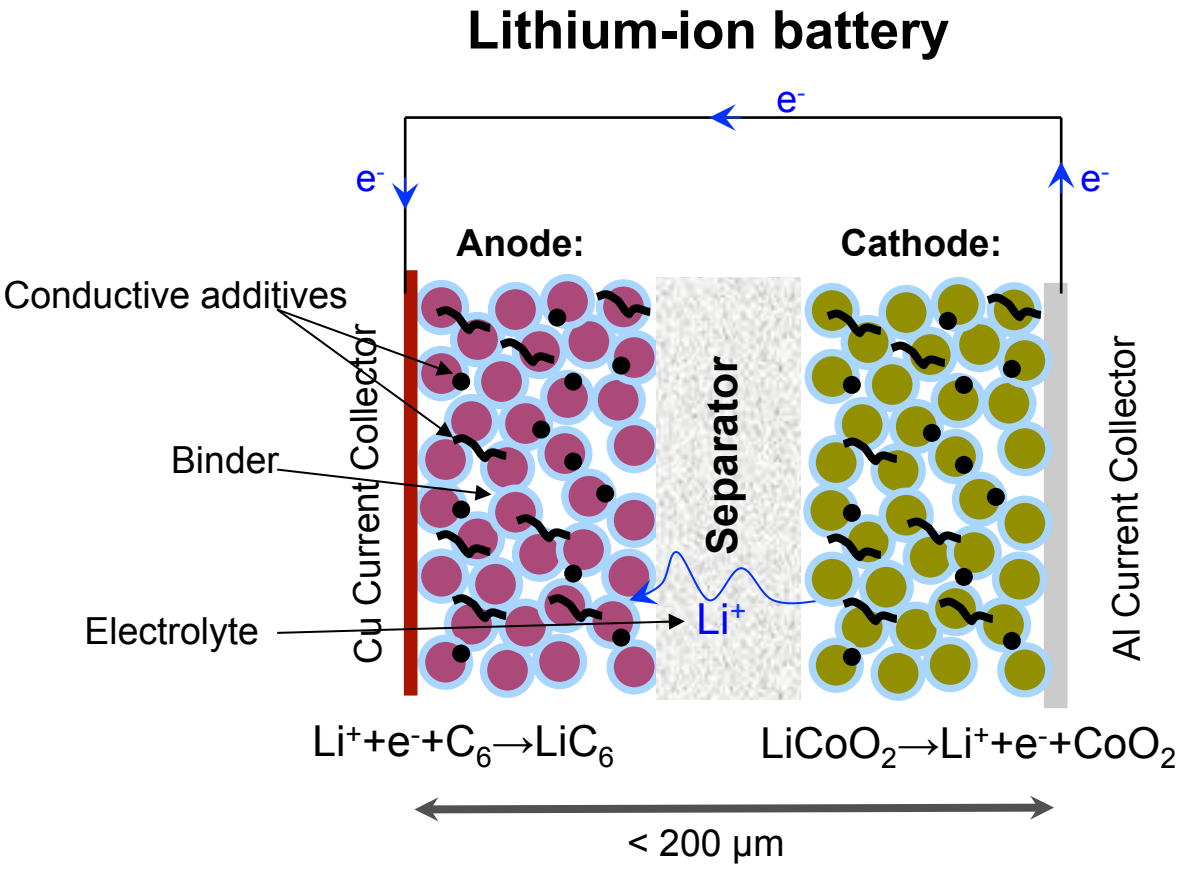
US DOE Synchrotron Facility
LBNL

Computation Facility



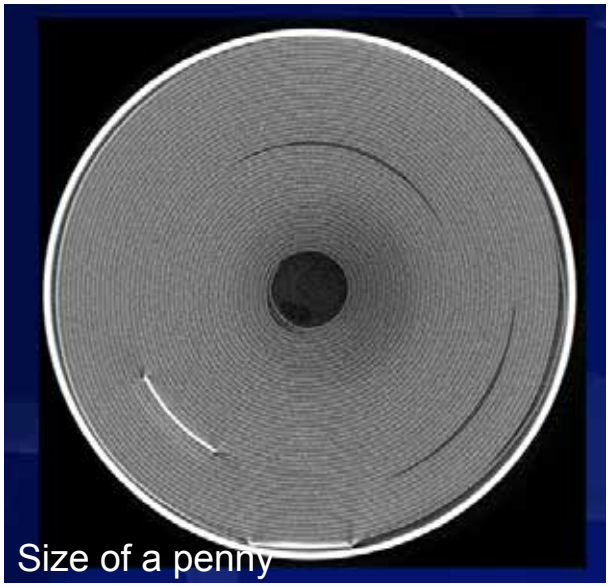
US DOE Computation User Facility
LBNL

Modern Li-ion Battery



Innovation can occur via new material development

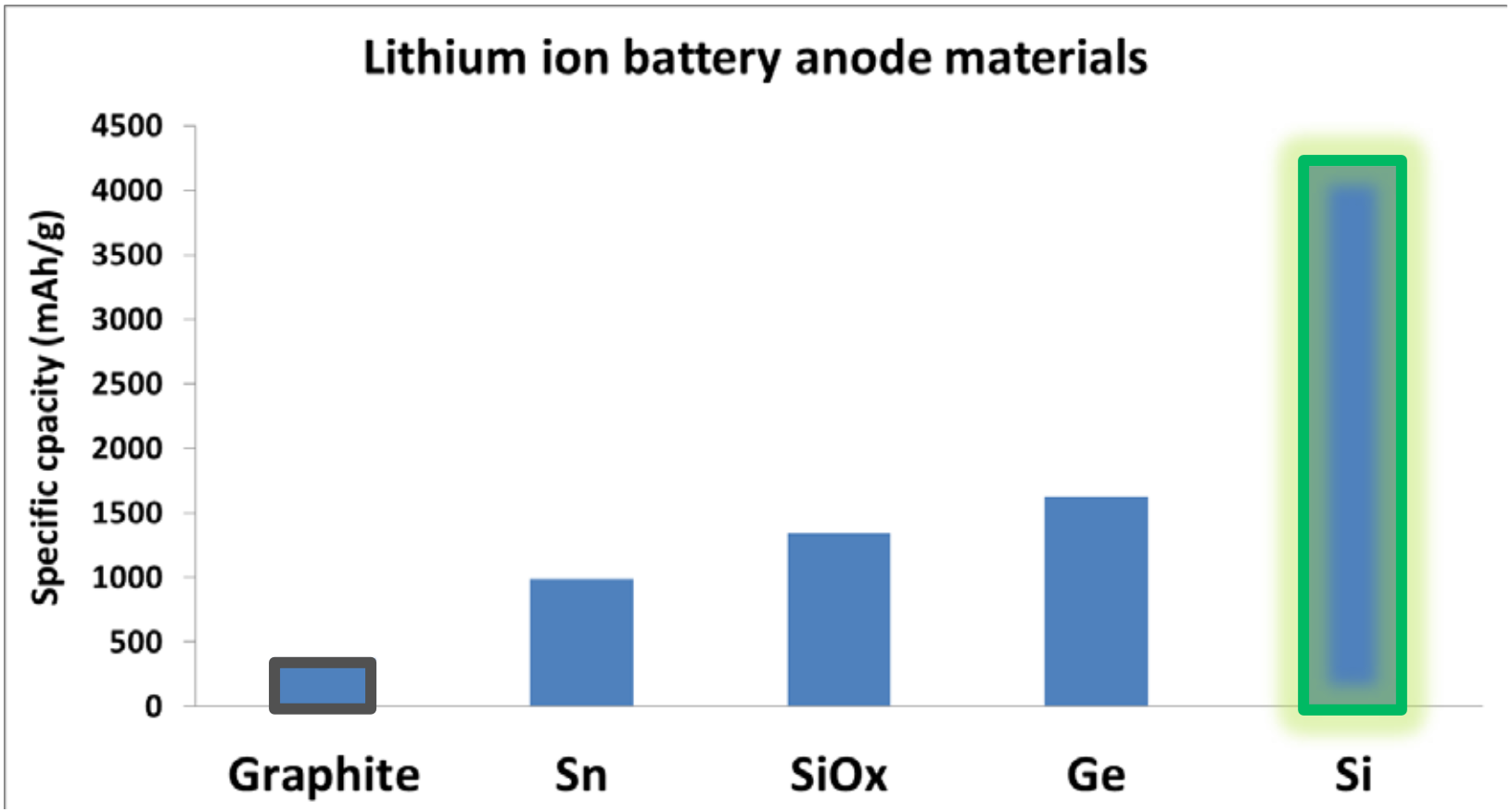
Spirally Wound Cell



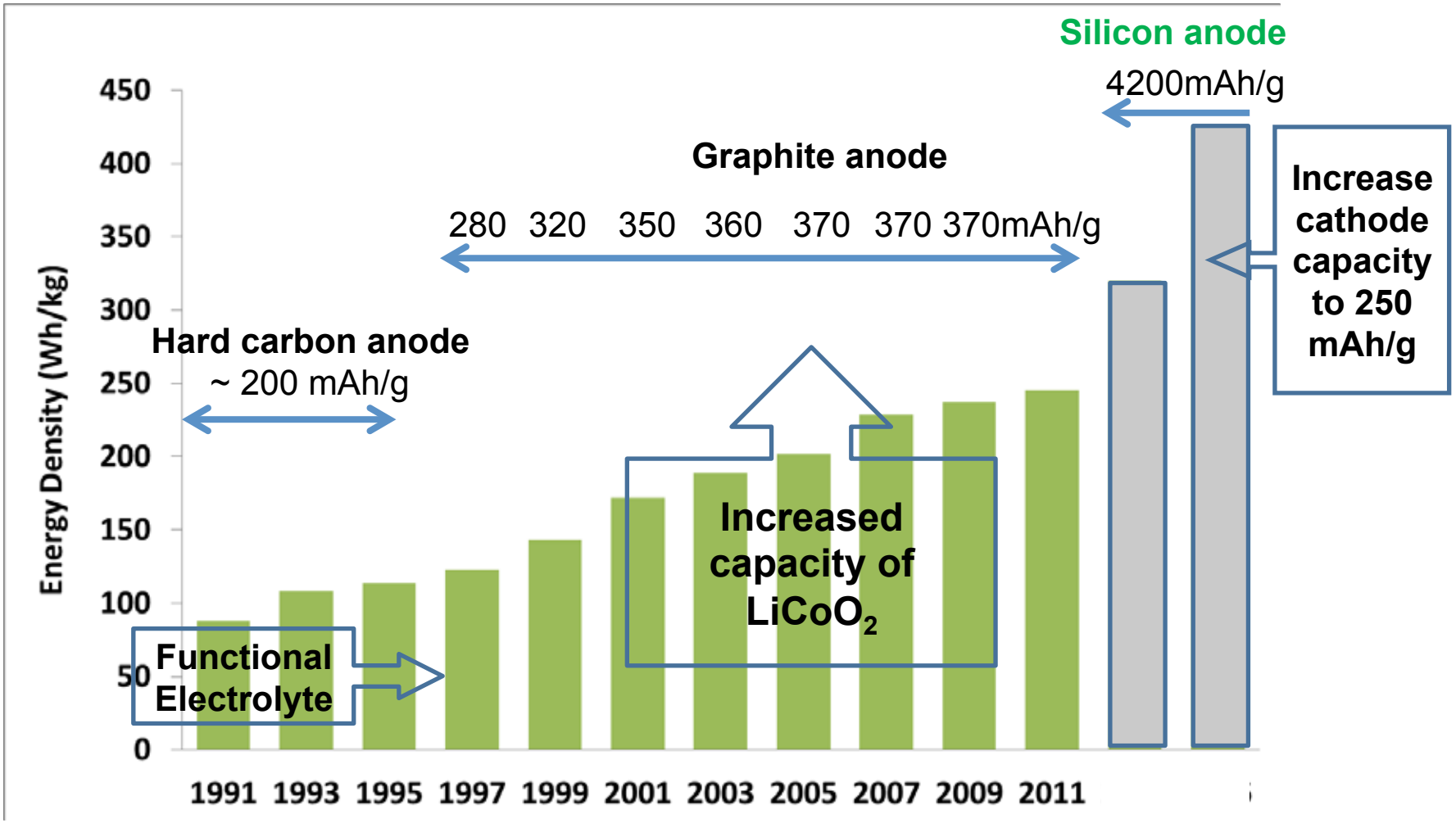
Prismatic Cell

Cylindrical Cell

Anode Materials Option



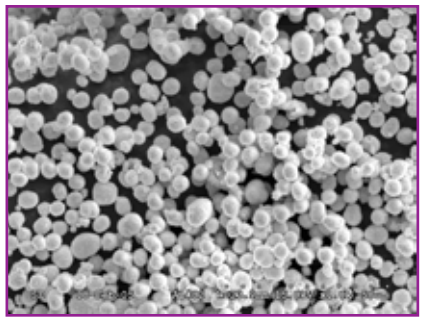
Improvement of Lithium ion Battery with Silicon Anode



A Quick Look at a traditional Composite Electrode

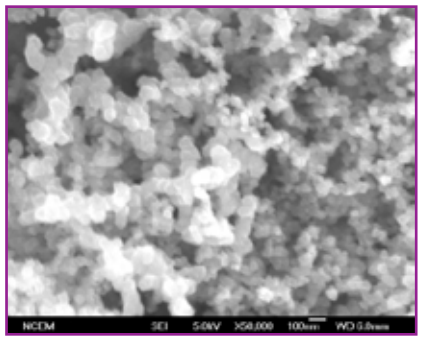
Materials

Active material



Ave. diam.: 10 μm
Surface area: 1 m^2/g
Conductor or semi conductor
Scale bar: 10 μm

Acetylene black (AB)



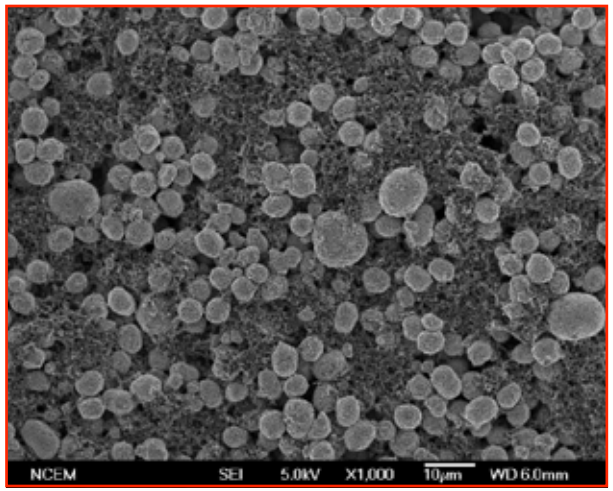
Ave. diam.: 50 nm
Surface area: 60.4 m^2/g
Conductor

Scale bar: 100 nm

Polymer Binder
Polyvinylidene difluoride (PVDF)

Insulator

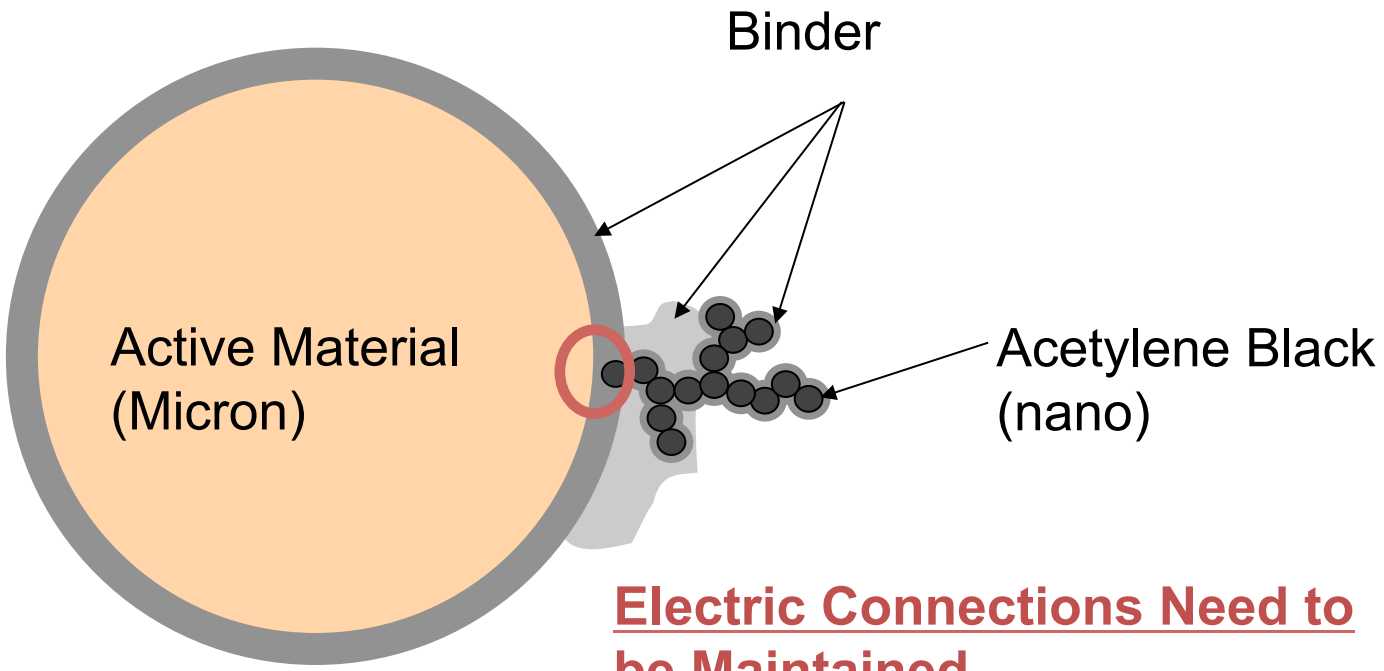
Electrode



Scale bar: 10 μm

Normal Composition (by weight):
Active material: 85%
AB: 5%
PVDF polymer binder: 10%

The Conditions for the Electrode to Function

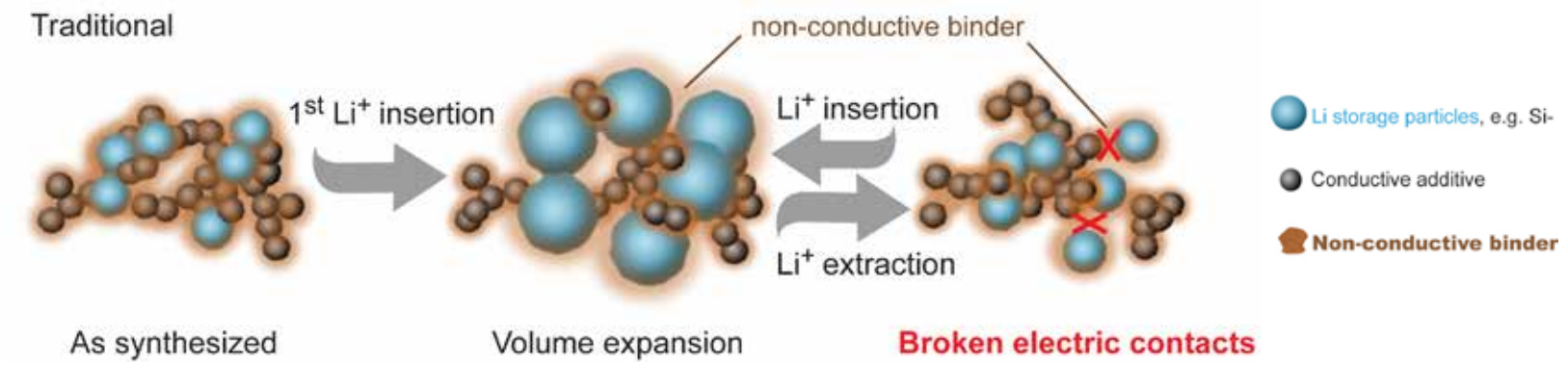


Electric Connections Need to be Maintained

The Challenges in a Si Electrode and Solution

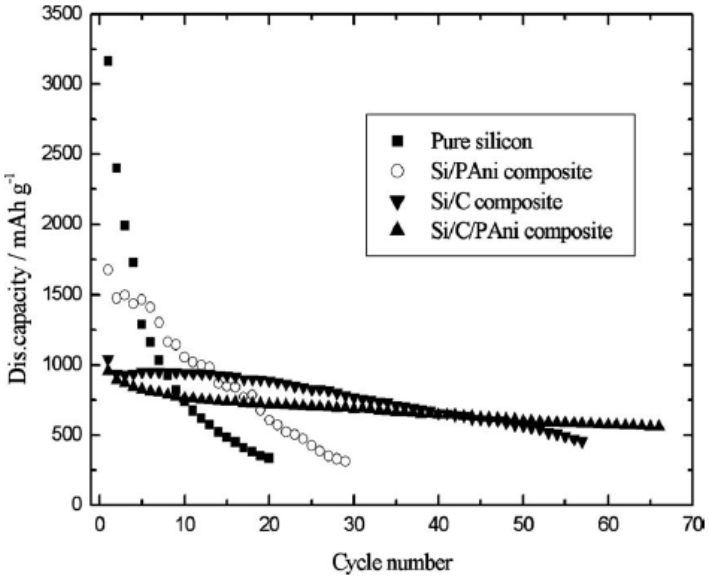
Schematic of electrode nanoscale structure

Non-conductive binder



Conductive Polymer Si Electrode

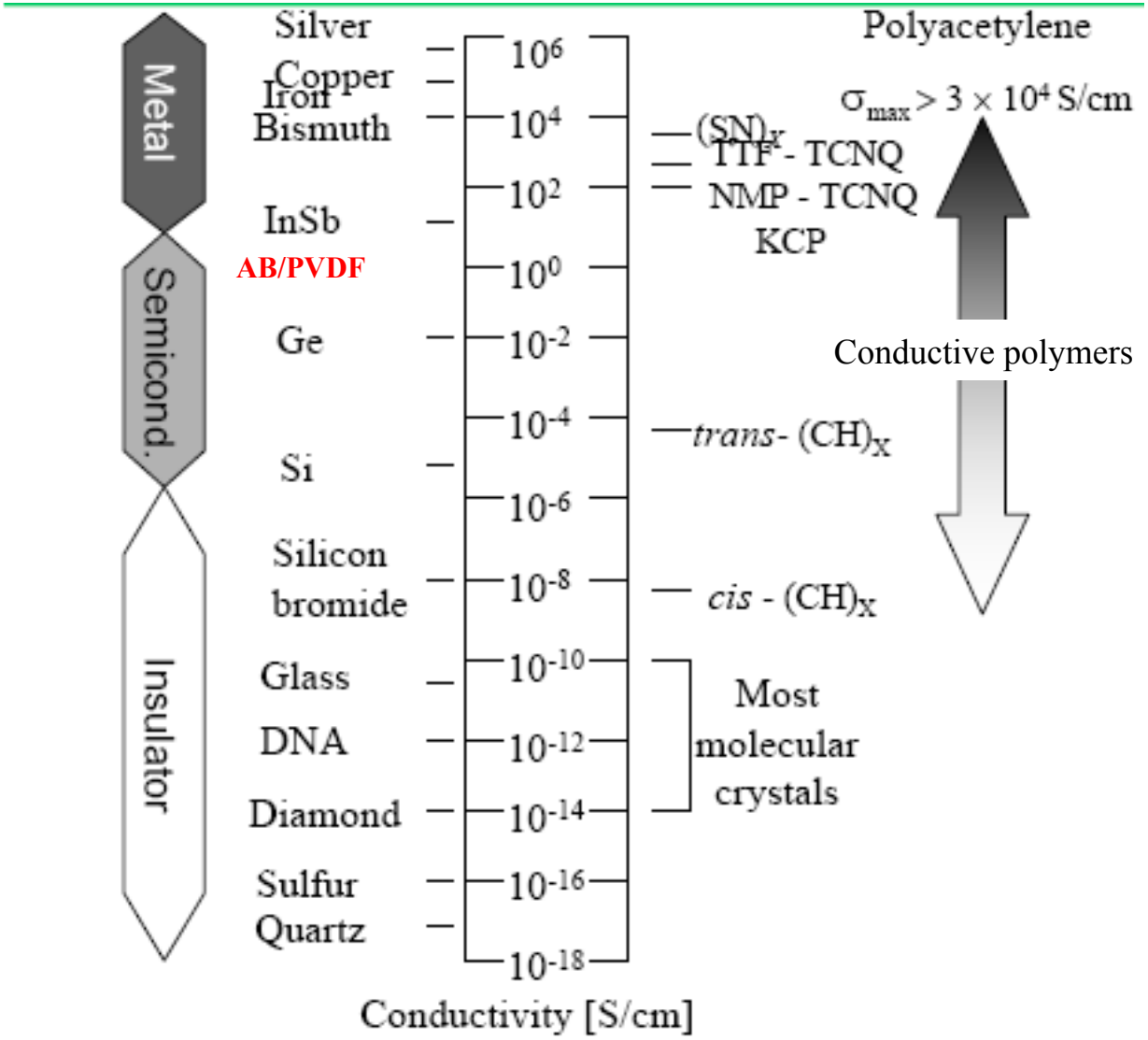
Theoretical capacity Si is 3500-4200 mAh/g



Literature result, 2005

Where does 2500 mAh/g go?

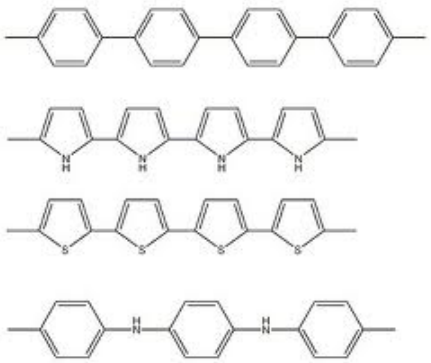
Conductivities of Materials



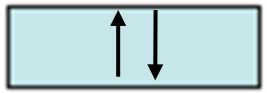
Formation of Polarons in Conjugated Molecule

Insulator

LUMO



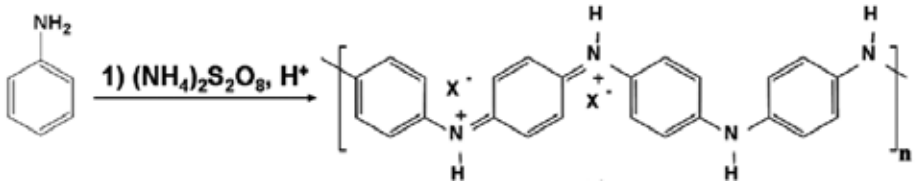
HOMO



Neutral

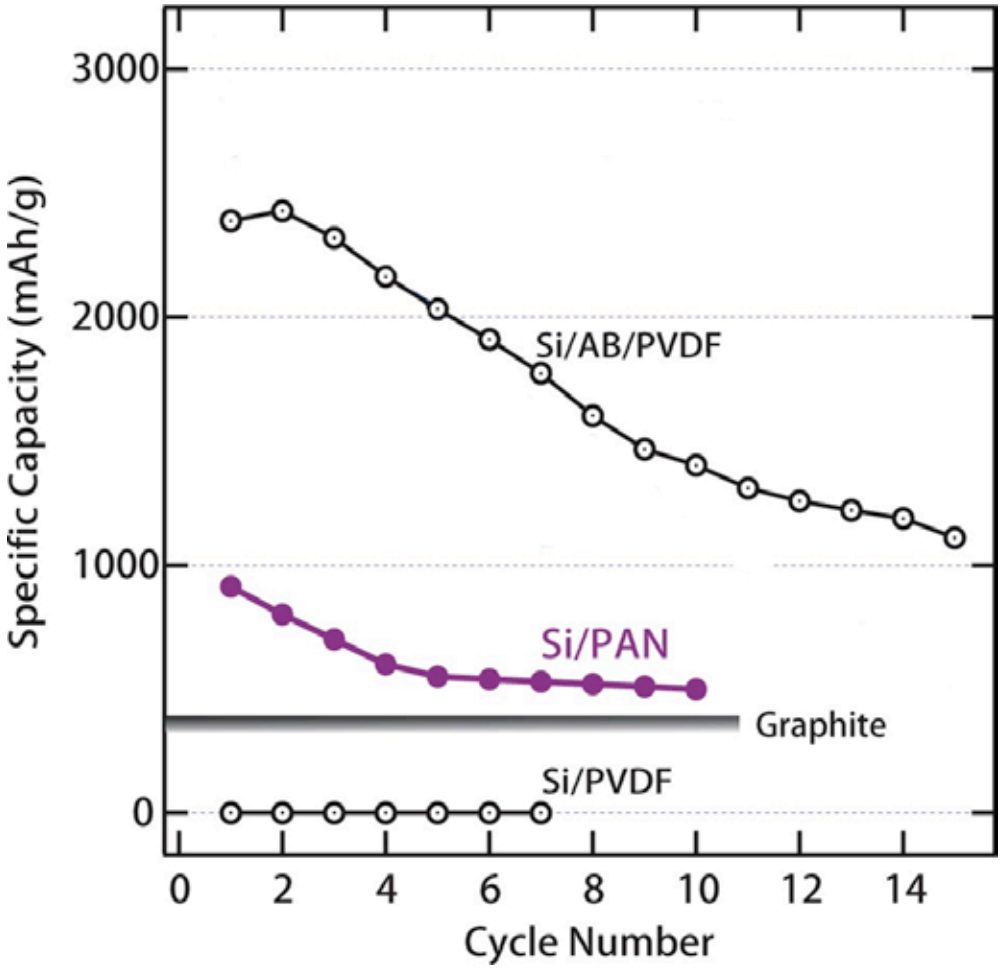
Polyaniline in the Negative Electrode Process

Commercial PAN product



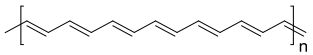
Emeraldine salt.
Oxidative (anodic) doped, conductive.

Electrode Performance Matrix with Nano-Si

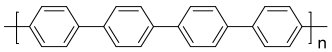


Rational Design of Conductivity in Polymer for Si Anode

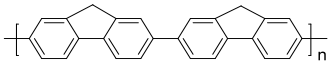
Choice of negative electrode polymer



polyacetylene: insoluble



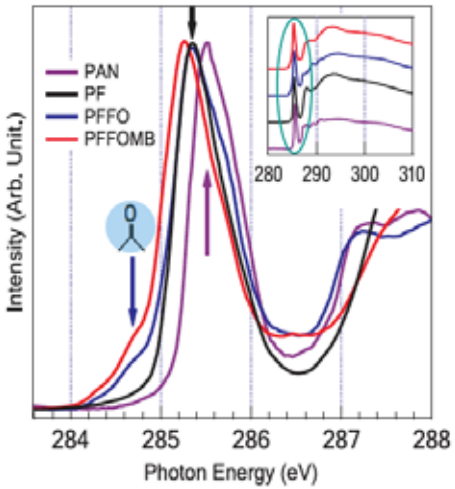
polyphenylene: insoluble



Polyfluorene

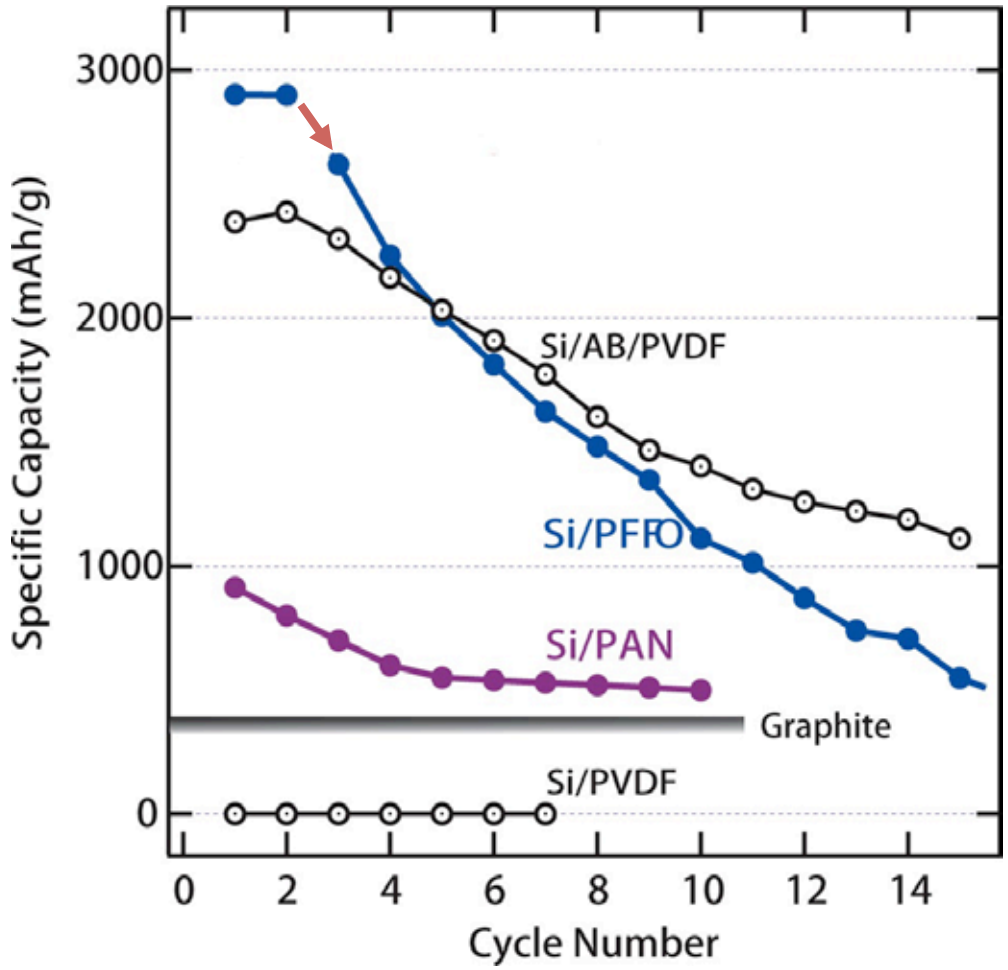
Chemically easy to modify

ALS XAS Characterization



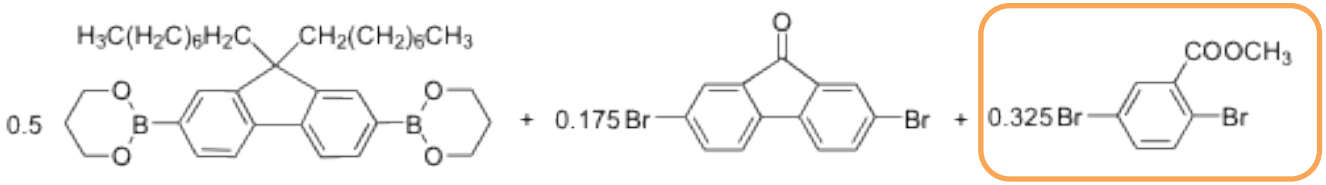
Wanli Yang, LBNL

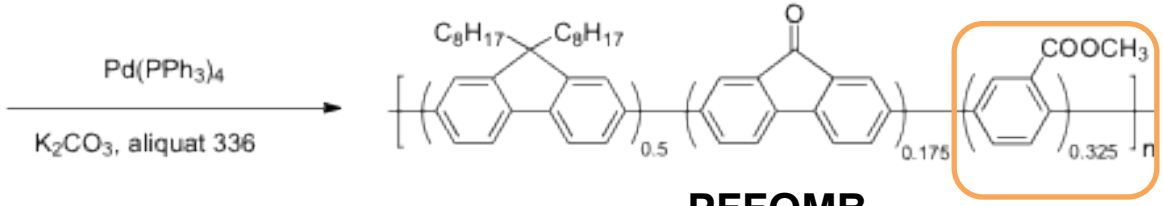
Cycling Performance of Commercial Si Nanoparticle with PFFO Conductive Polymer



Improve Adhesion of the Conductive Polymer Binder

Synthesis





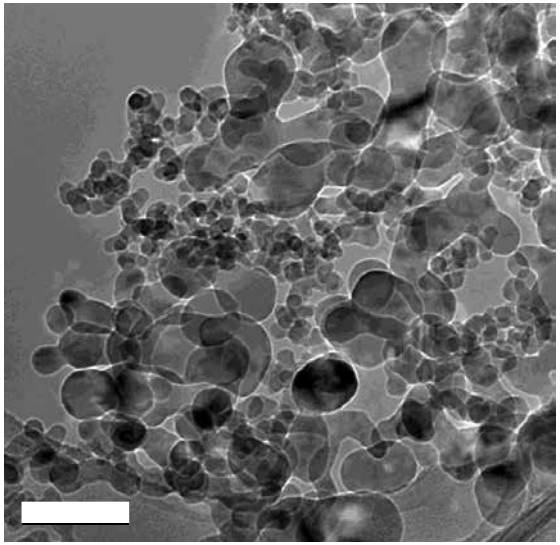
Better Adhesion

PFFOMB

Commercial Si Nanoparticle/Conductive Binder Composites

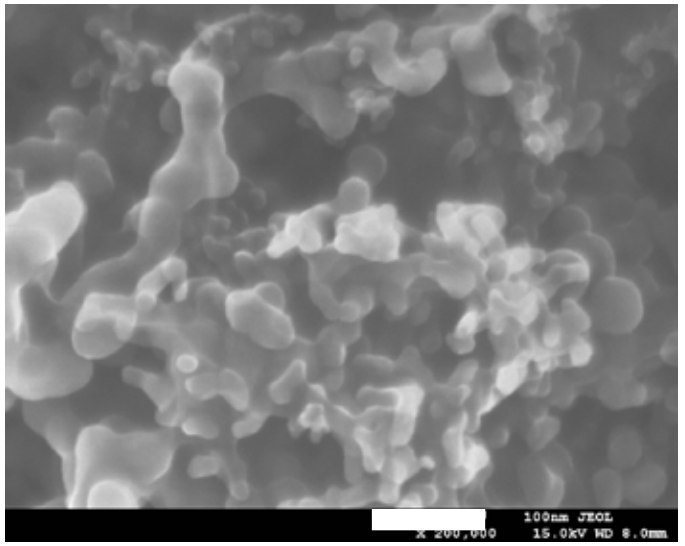
Powder & Electrode Images

Si Particles-TEM



Commercial source material.

Electrode-SEM

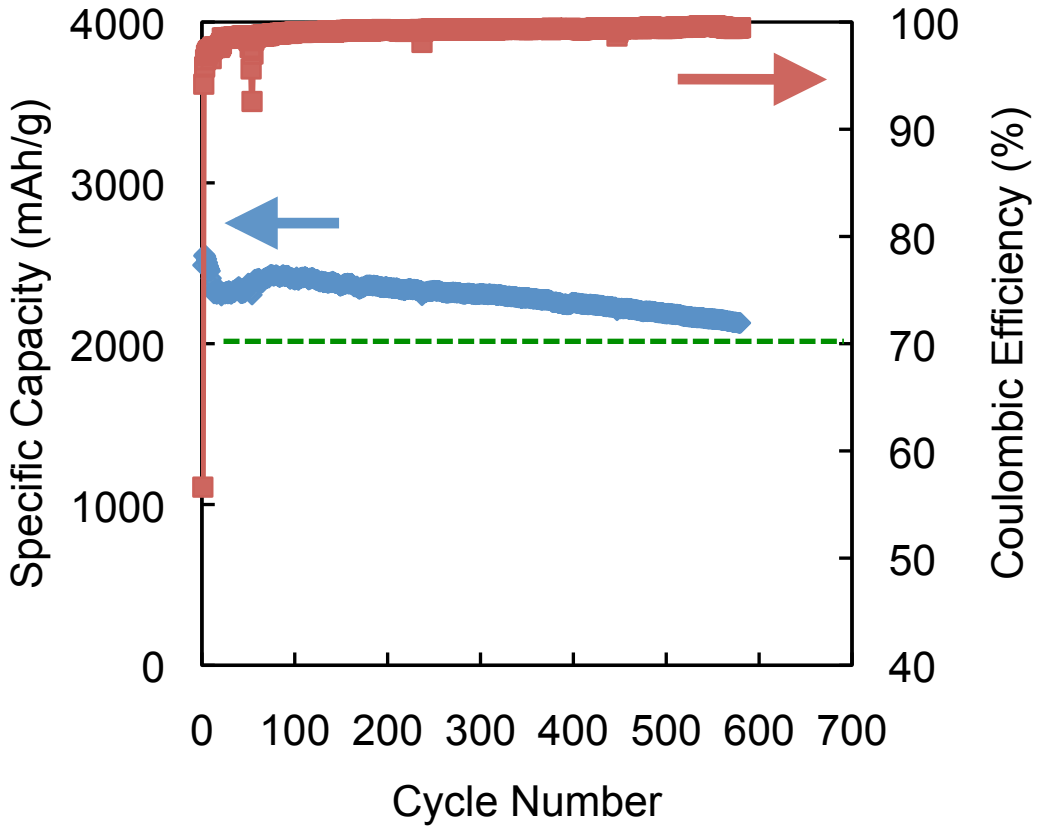


Scale bars 100 nm

Si/conductive binder Composition.

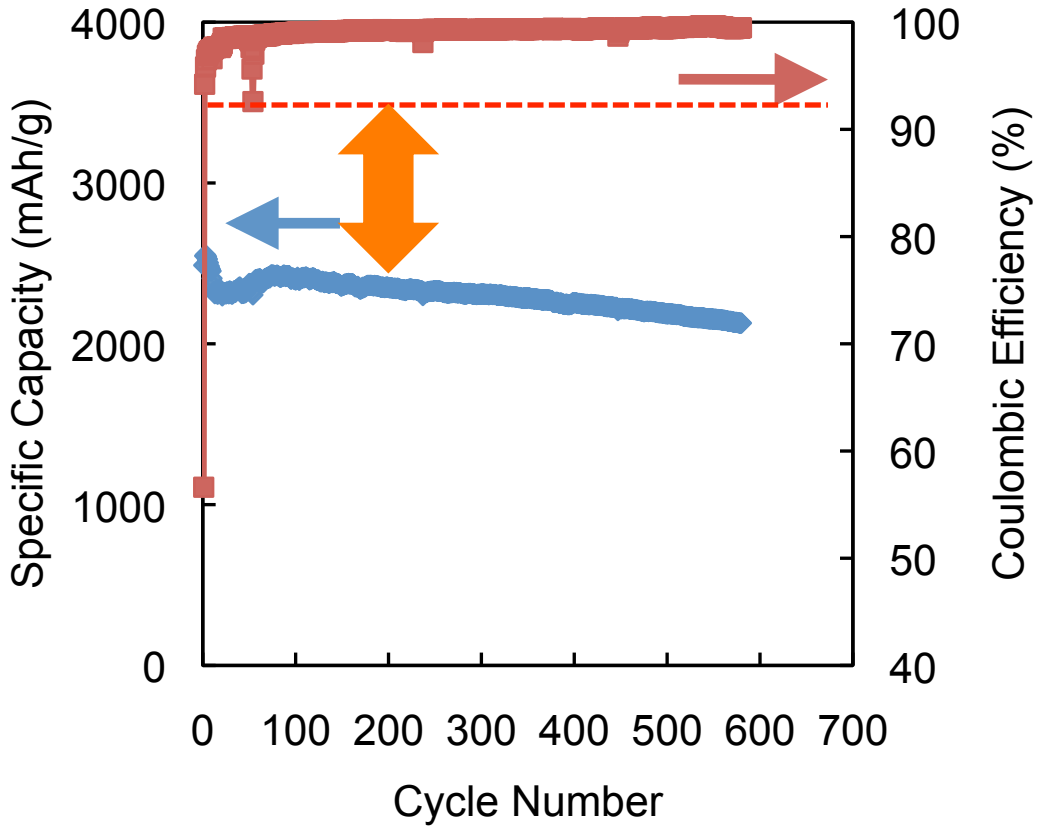
- Si 66% (by weight)
- Conductive polymer 34%

Cycling Performance Comparison



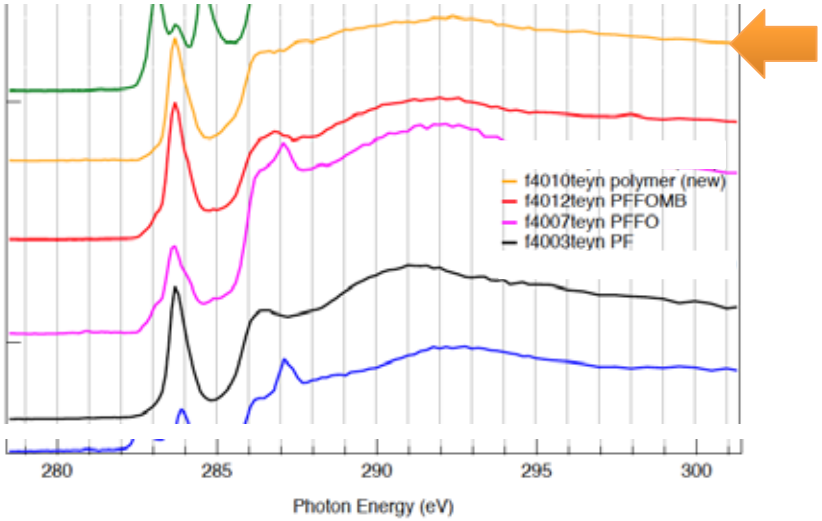
Electrode composition by weight
Si 67%, PFFOMB binder 33%
No conductive additives
Deep cycling 1V-0.01V

Where Does 1000 mAh/g Go?

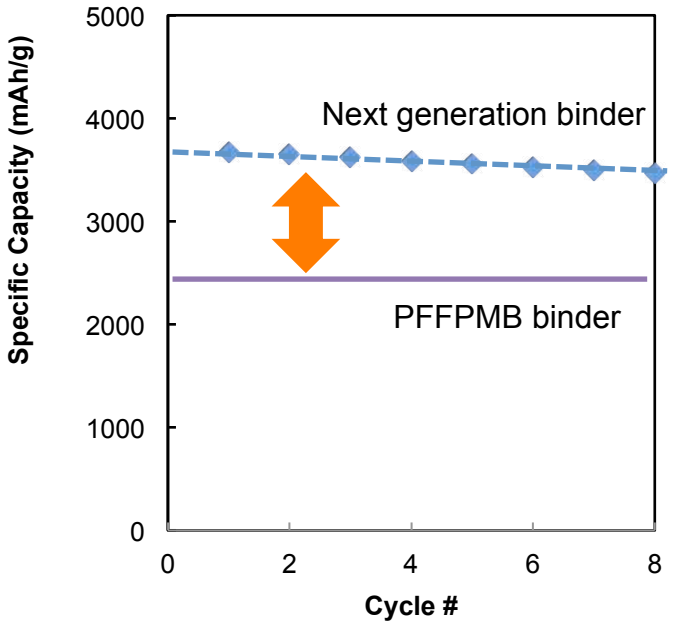


A New Polymer Binder Leads to Full Si Capacity Cycling

XAS



Si Cycling – Discharge



67% Si nanoparticles
34% polymer binder

Conclusions

•Conductive polymer binder is a viable approach to enable Si material for lithium ion anode application.

•The critical property of the conductive binder has to be compatible with lithium ion negative electrode, and in situ cathodically doped during lithium ion insertion process.

•Adhesion is important to the Si electrode performance

Acknowledgements

BATT program, OVT Office, US DOE

Thank You for Your Attention!