Supporting information

High Capacity Silicon/Graphite Composite as Anode for Lithium-Ion Batteries using low content amorphous Silicon and Compatible Binders

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Experimental

Fourier Transform Infrared spectroscopy (FTIR)

Attenuated total reflectance (ATR) FTIR spectra were taken on Nicolet 6700 from Thermo Scientific. Single bounce diamond was used for the ATR element. The frequency was measured from 550 cm^{-1} to 4000 cm^{-1} for 256 times. No sample preparation was required for binders and silicon, except PEI. PEI was rigid and big crystals that could not fit into the ATR element. As a result, the PEI was dissolved in NMP and fully dried in convection and vacuum oven in clean Petri-dish. As a result, fine PEI film is obtained that can be measured for ATR FT-IR. Silicon powder with binder was washed with water or NMP to find the interaction of the binder, similar method was tried by Kovalenko et al.[1] The silicon powder is mixed with the binder in 1:1 ratio and washed; NaCMC and NaPAA were washed with water, and PVDF and PEI were washed with NMP. Mixture of silicon and binder was mixed with water or NMP, sonicated, vortexed, and centrifuged. Supernatant was discarded and the silicon precipitates was washed, vortexed,

and centrifuged 2 more times. The washed silicon powder were dried in vacuum oven at 85 ^{o}C for 1 hr and tested on FR-IR.

Results and Discussion

FR-IR

Figure S 4 to Figure S 7 shows the FT-IR spectra of the binders, the silicon powders and the washed silicon. The top layer of the FR-IR spectra is the finger prints of the binders tested in this paper. The middle spectra are the washed silicon with different binders and the bottom spectra is the Si-200h as a reference to the other spectra. Kovalenko et al.[1] have tried the same method with alganic acid, and found the strong interaction with the binder and the silicon. However, in the present experiment no conclusive results could be observed.

Ternary composition diagram

The diagram was obtained with the following equations and parameters to achieve the composition diagram.

Equations

The maximum volume change (V_{max})

$$V_{max} = f_{Si}\, V_{Si} + f_{Carbon}\, V_{Carbon}$$

The total specific capacity (C_{tot})

$$C_{tot} = f_{Si} C_{Si} + f_{Carbon} C_{Carbon}$$

Since we are dealing with the composite in fractions

$$f_{Si} + f_{Carbon} + f_{Binder} = 1$$

C_{Si}: Specific Capacity of Silicon, 4200 mAh g^{-1}

C_{Carbon}: Specific Capacity of Carbon, graphite in this case, 372 mAh g^{-1}

V_{Si}: Maximum volume change when fully lithiated, 297%

V_{Carbon}: Maximum volume change of Carbon, 12%

These parameters are obtained from Nazri et al.[2]

According to the parameters and equations, the constant volume and capacity lines with different fraction of the composites are drawn in the diagram. The diagram is used to understand the composite ratios according to the total specific capacity and volume expansion as a reference.

Figures

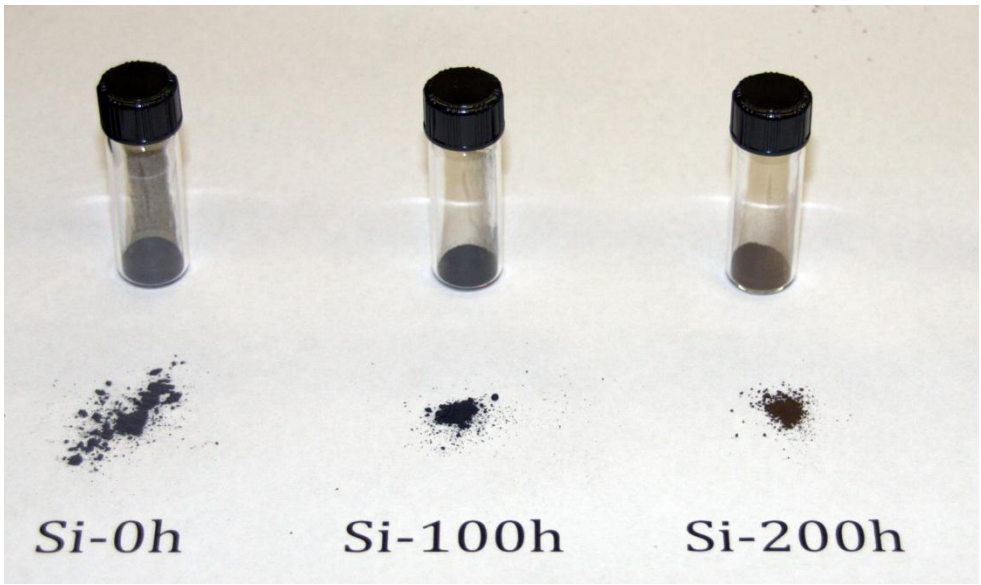

Figure S 1 Color changes of the silicon powders as a function of the ball milling time

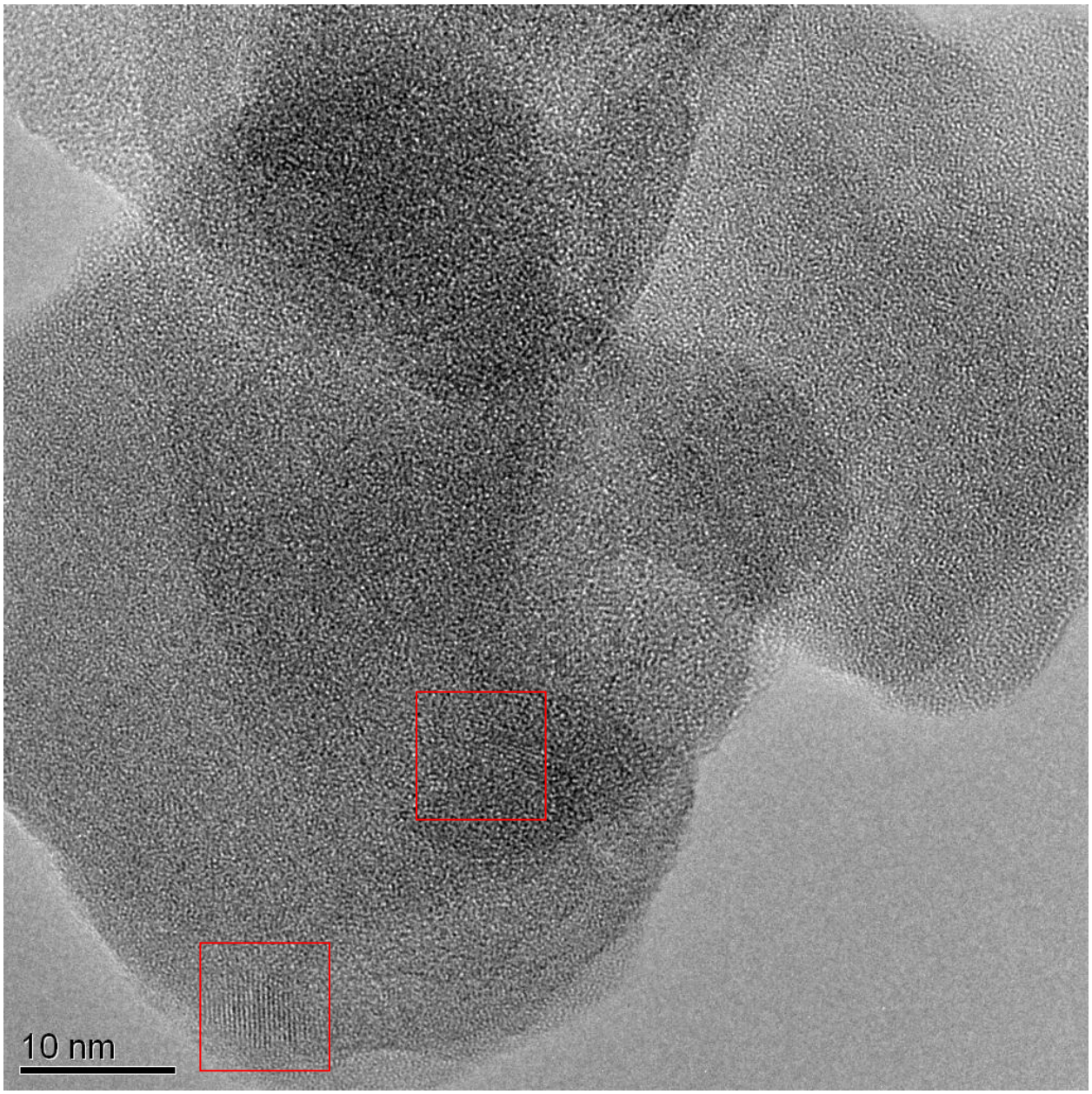

Figure S 2 High resolution TEM of Si-200h

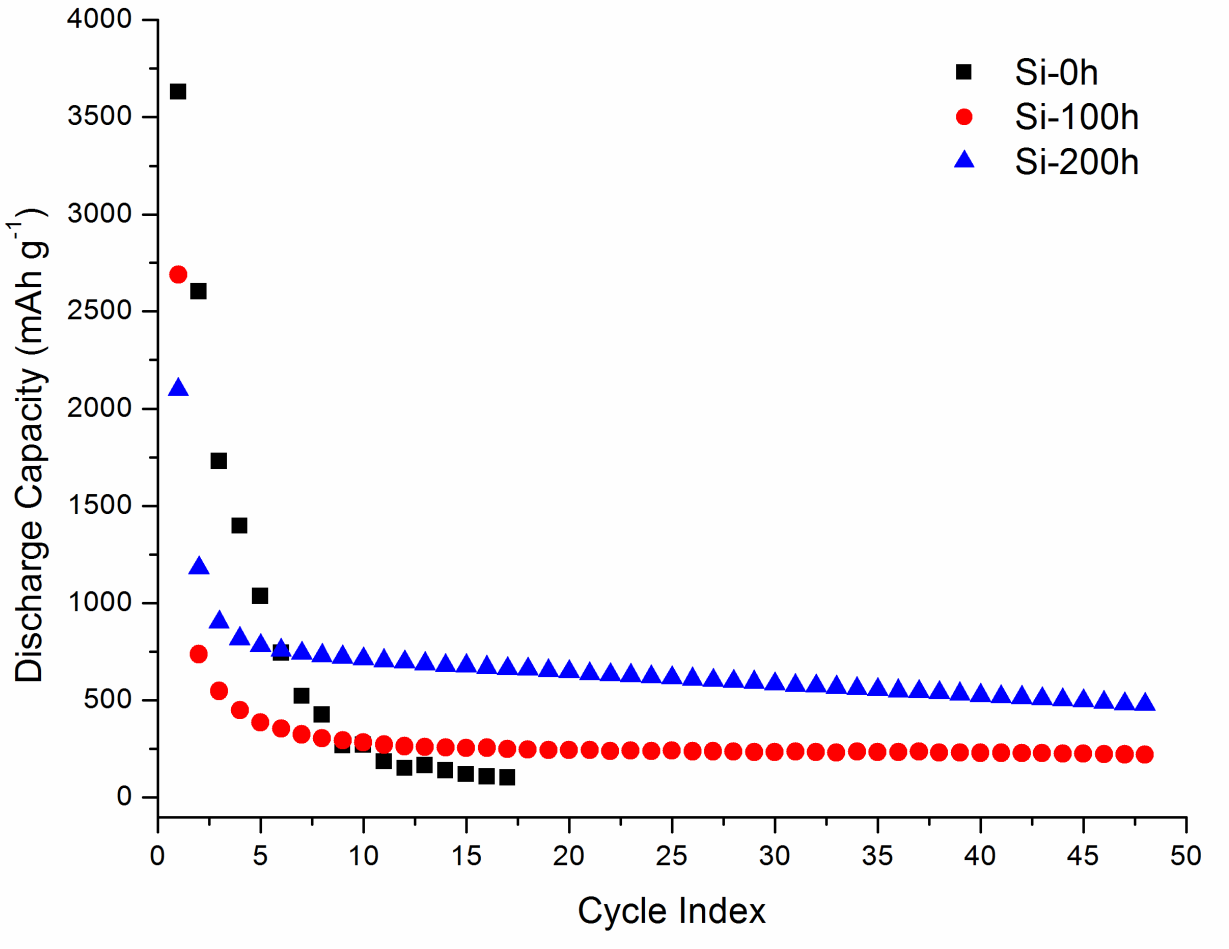

Figure S 3 Cycling performance of silicon, Si-0h, Si-100h, and Si-200h, cycled between 5 mV to 1.5V versus Li/Li^+ at C/12 (350 mA g^{-1}) using NaCMC binder

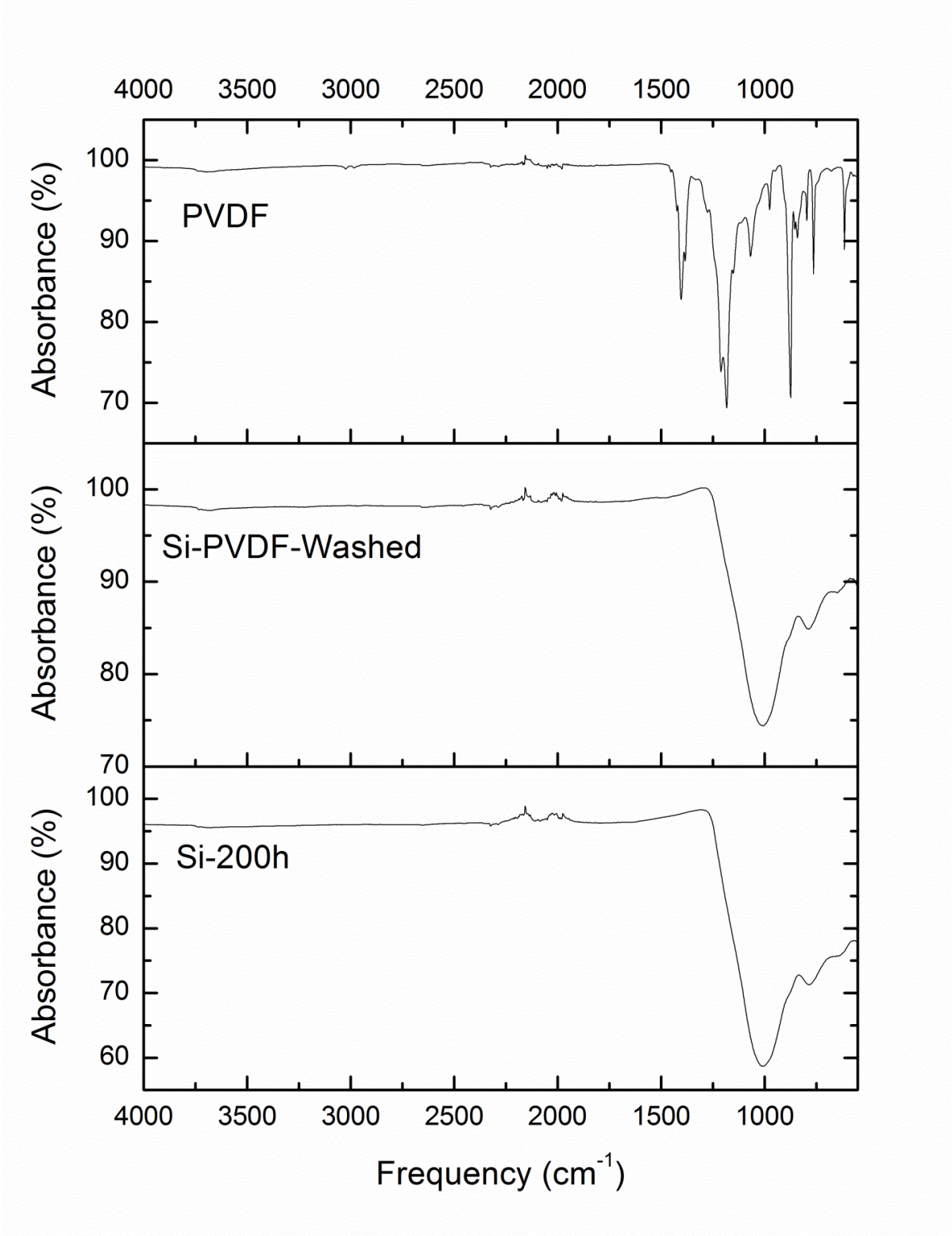

Figure S 4 IR spectra of Si-200h, PVDF and their 1:1 composite.

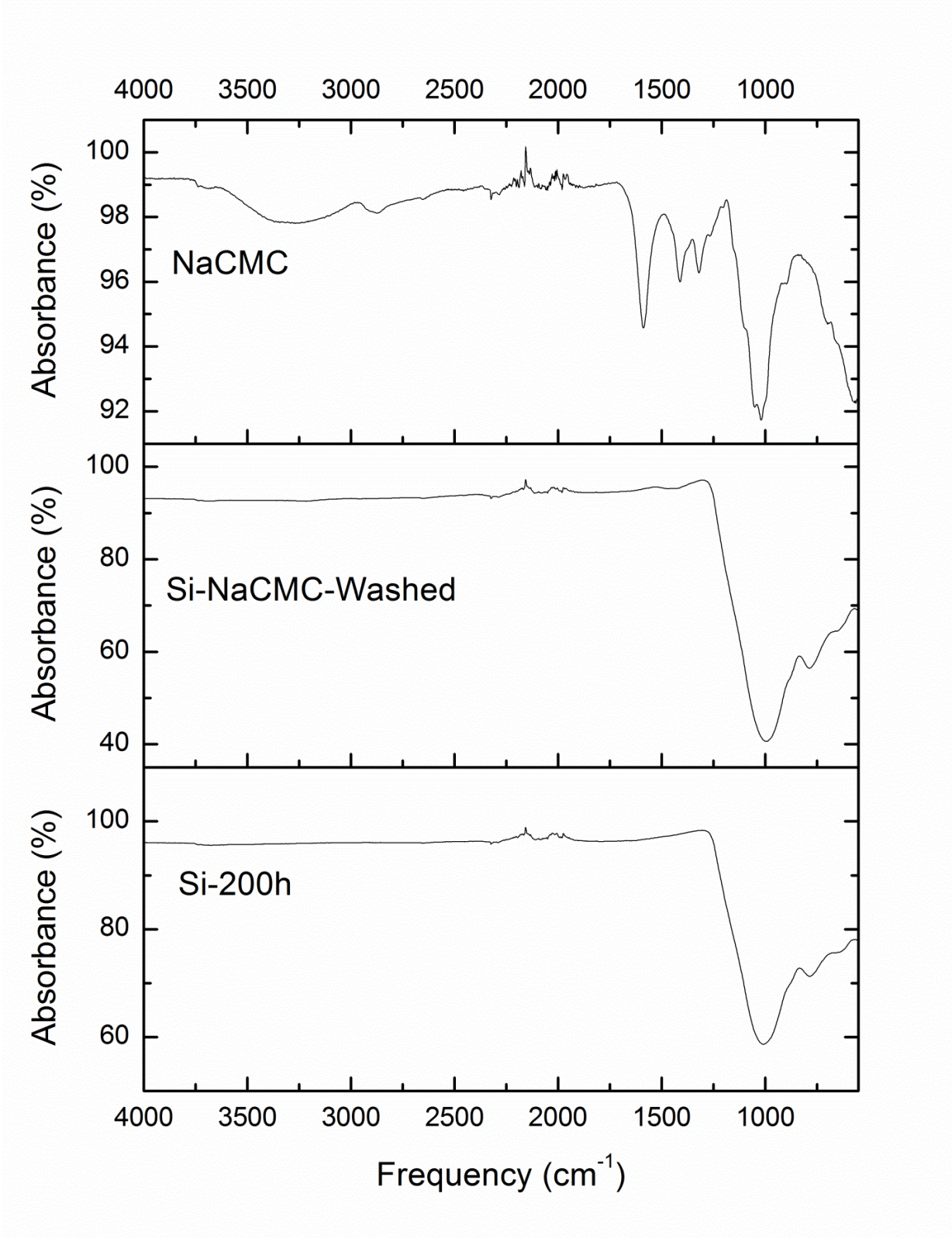

Figure S 5 IR spectra of Si-200h, NaCMC and their 1:1 composite.

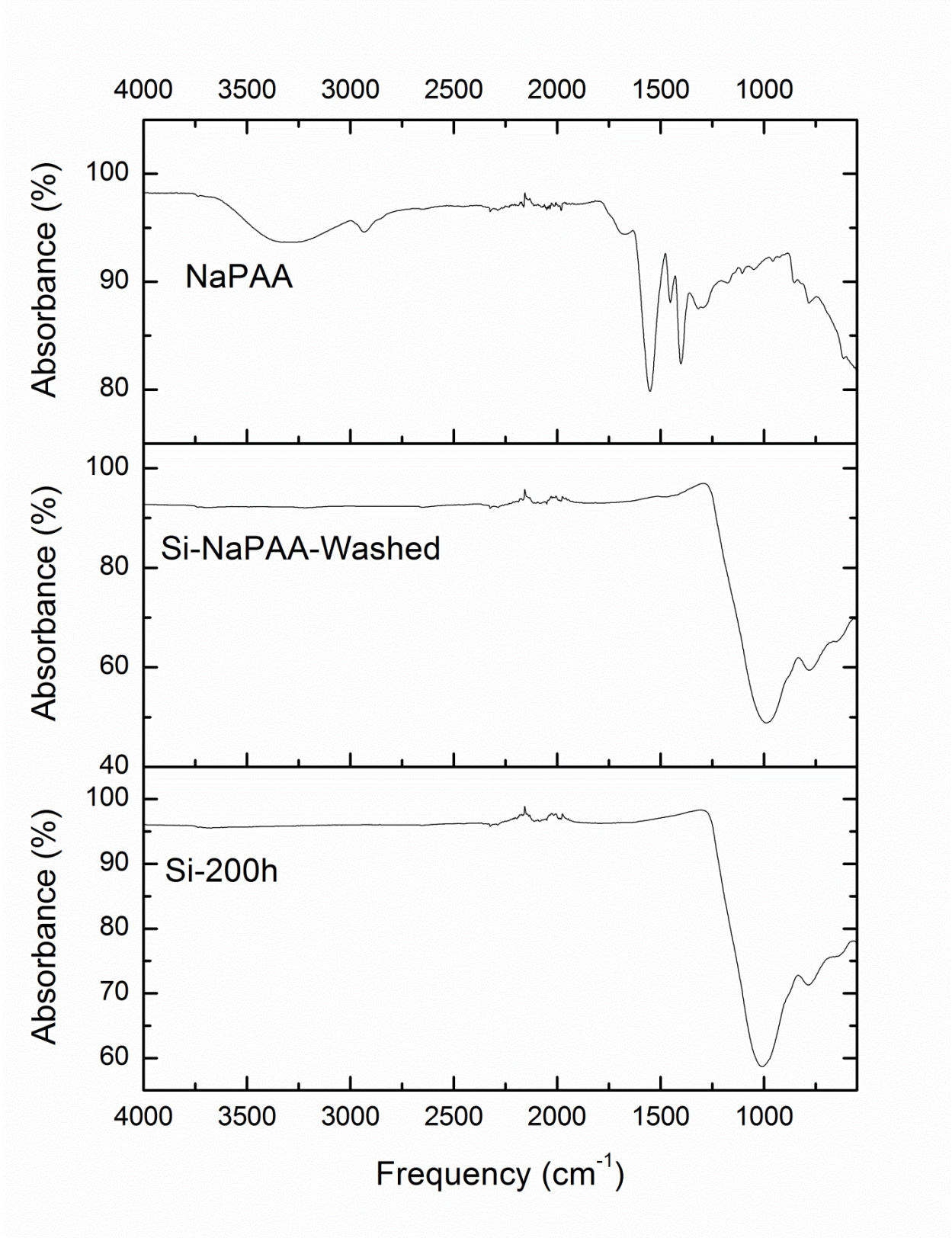

Figure S 6 IR spectra of Si-200h, NaPAA and their 1:1 composite.

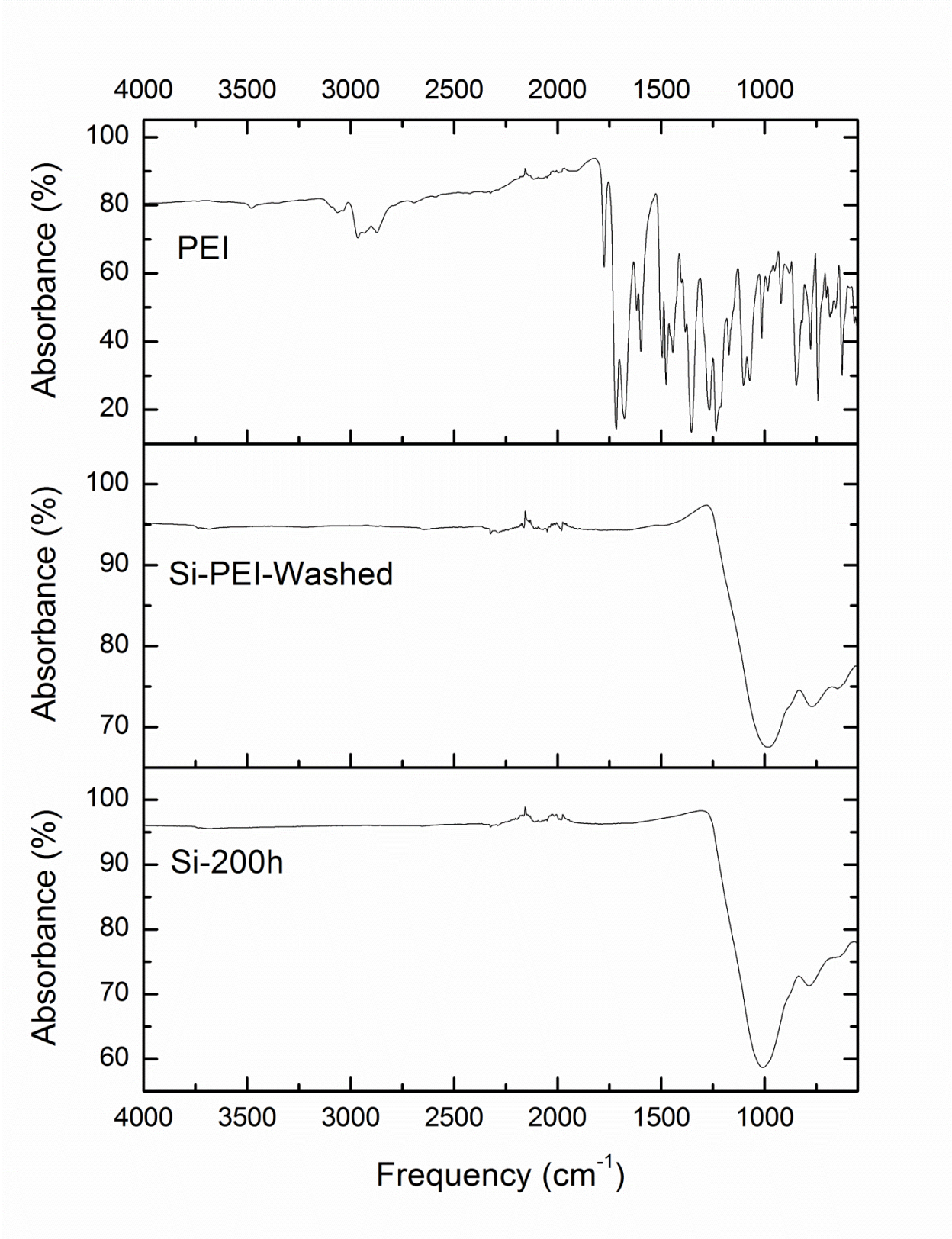

Figure S 7 IR spectra of Si-200h, PEI and their 1:1 composite.

Reference

1. I. Kovalenko, B. Zdyrko, A. Magasinski, B. Hertzberg, Z. Milicev, R. Burtovyy, I. Luzinov and G. Yushin, *Science*, 2011.
2. G.-A. Nazri and G. Pistoia, *Lithium Batteries: Science and Technology*, Kluwer Academic Publisher, Boston, Dordrecht, New York, London, 2003.