

The Versatile Si/P System as efficient anode for Li and Na-batteries: Understanding of an original Electrochemical Mechanism by a Full XRD-NMR Study.

Gaël Coquil [†]; Bernard Fraisse [†]; Nicolas Dupré ^{‡, †, *}; Laure Monconduit ^{†, §, ‡, *}

[†] Institut Charles Gerhardt, Université de Montpellier, 34095 Montpellier, France.

[‡] Institut des Matériaux Jean Rouxel (IMN), CNRS UMR 6502, Université de Nantes, 44322 Nantes Cedex 3, France

[§] Réseau sur le Stockage Electrochimique de l'Energie (RS2E), CNRS FR3459, 33 Rue Saint Leu, 80039 Amiens, Cedex, France.

^{*} ALISTORE European Research Institute, Université de Picardie Jules Verne, 80039 Amiens, France

Supporting information

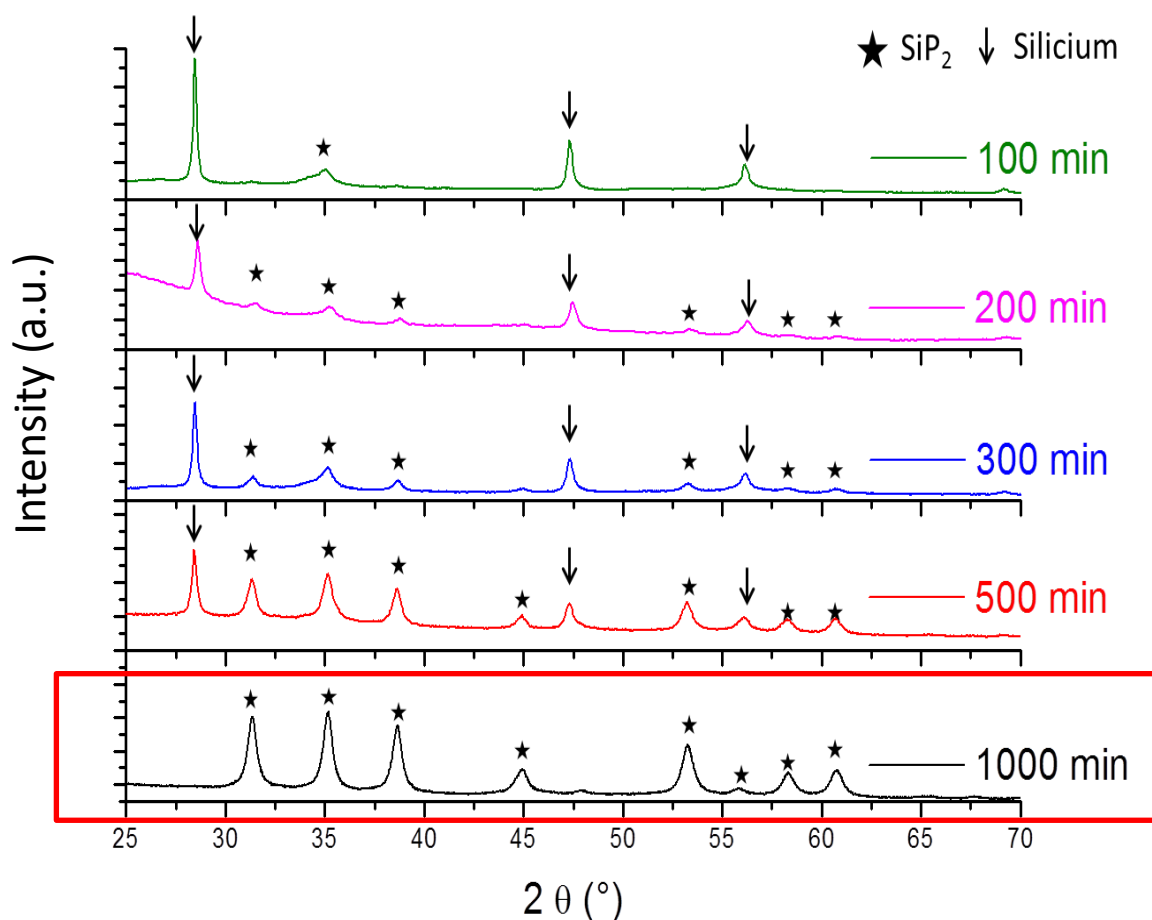


Figure S1: XRD after different duration of milling.

SiP_2 microparticles were prepared by ball milling of Si and red P powders. Figure S1 shows the XRD after various ball milling duration. An active-milling time of 16h of the stoichiometric mixture Si-2P allowed obtaining a complete reaction between Si and P. An intimate mixture Si/P in 1/2 composition was also prepared by a short grinding (15 min) for further electrochemical comparison.

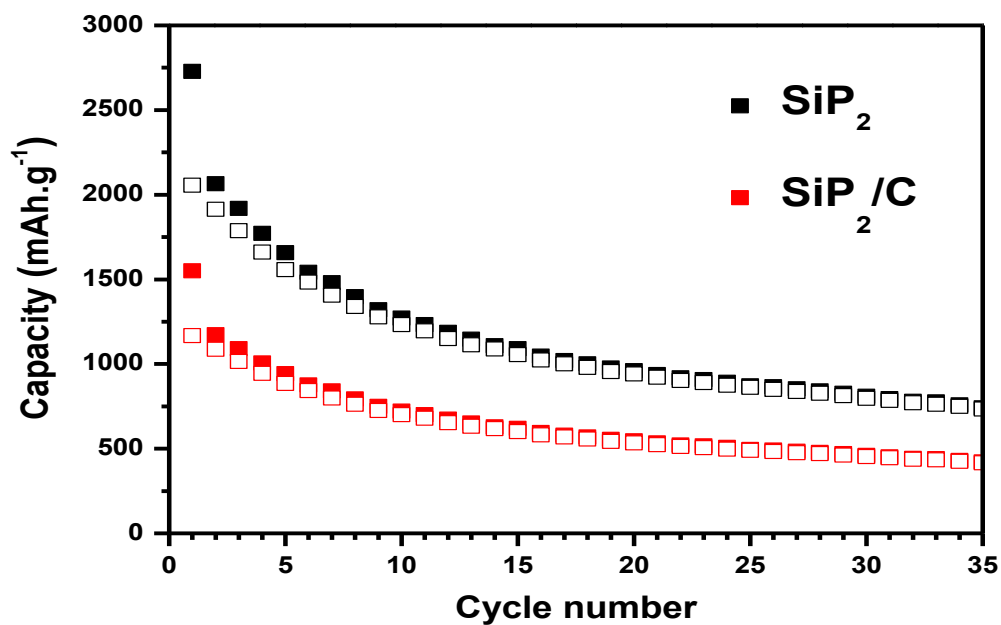


Figure S2: Capacity retention calculated for SiP₂ and SiP₂/C electrodes vs Li.

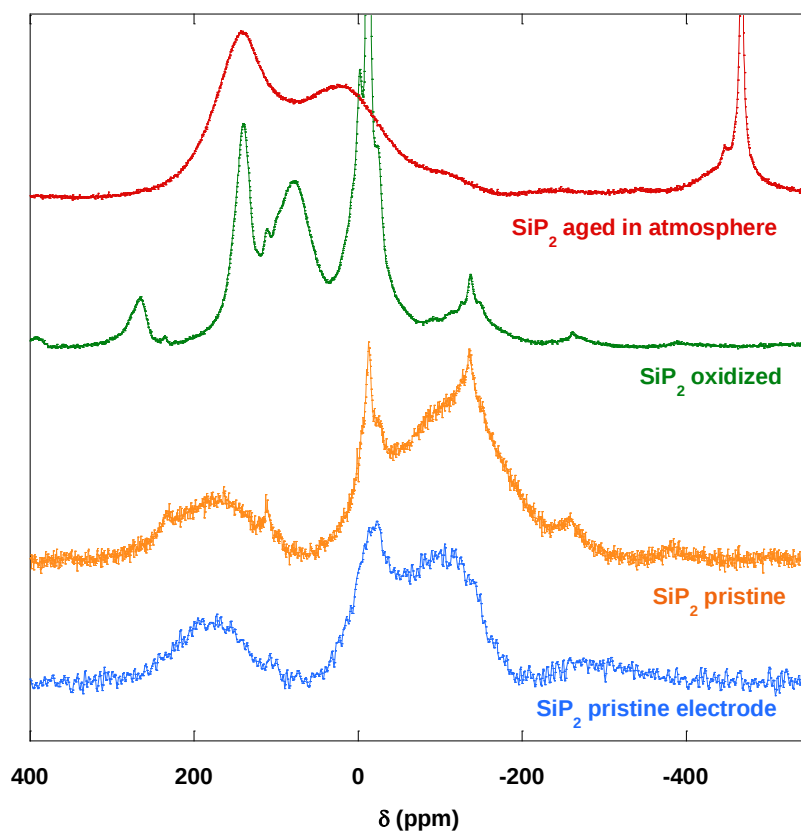


Figure S3 : ³¹P MAS NMR spectra of pristine SiP₂ (orange), SiP₂ electrode prior to cycling (blue), SiP₂ aged in ambient atmosphere (red) and SiP₂ after an oxidizing treatment (green)

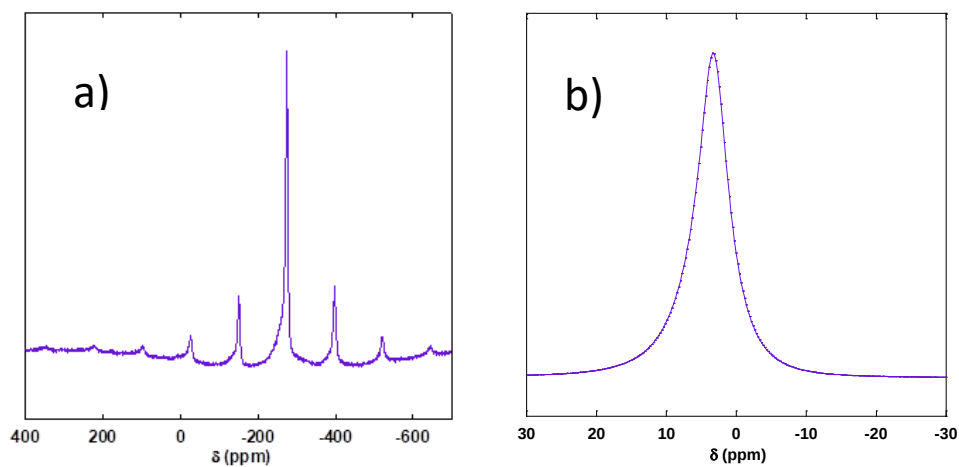


Figure S4: a) ^{31}P (left) and b) ^7Li (right) MAS NMR spectrum of Li_3P prepared by ball milling.

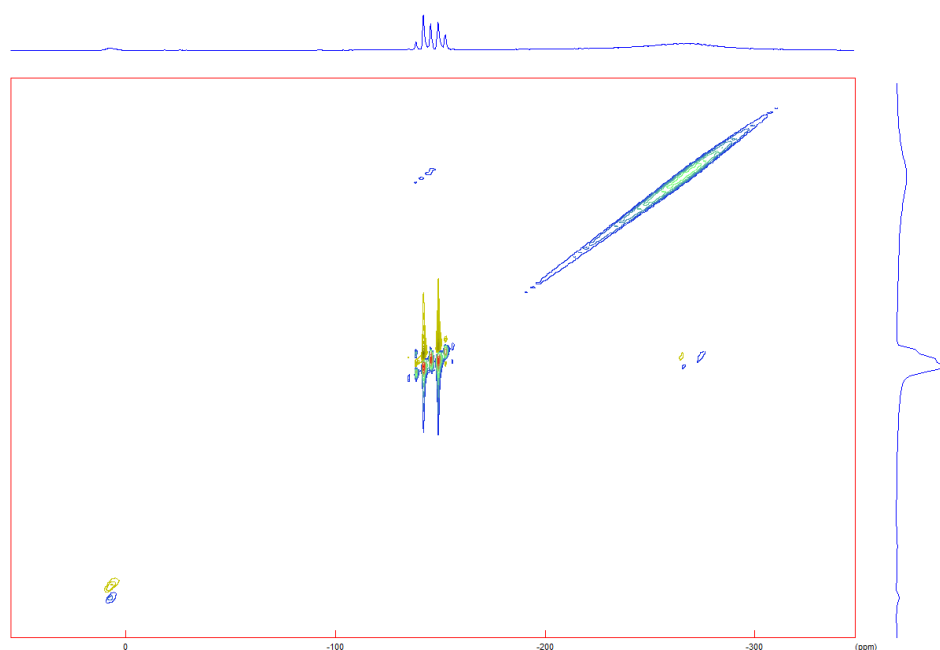


Figure S5: ^{31}P 2D NMR EXSY for an electrode cycled vs Li and stopped at the end of discharge.

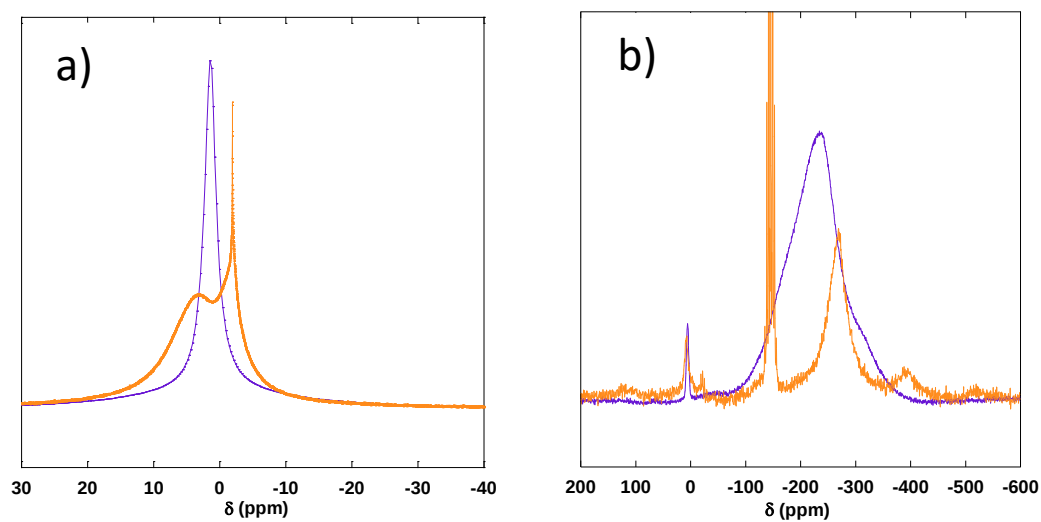


Figure S6 : a) ^7Li (left) and b) ^{31}P (right) MAS NMR spectra of the Li_5SiP_3 model ball milled sample (violet) and a SiP_2 electrode stopped at the end of the lithiation process (orange).

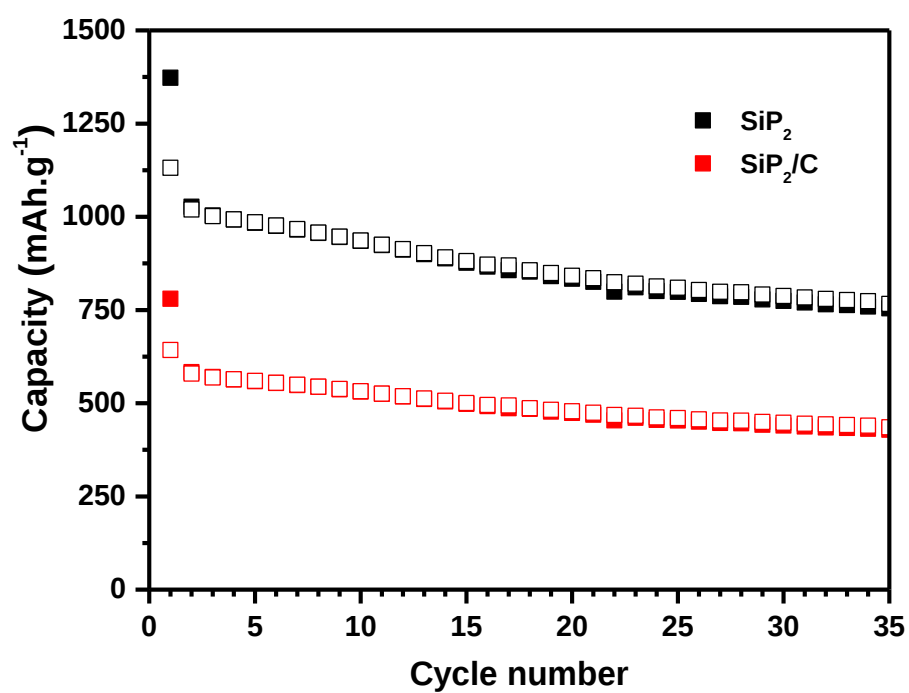


Figure S7: Capacity retention calculated for SiP_2 and SiP_2/C electrodes vs Na

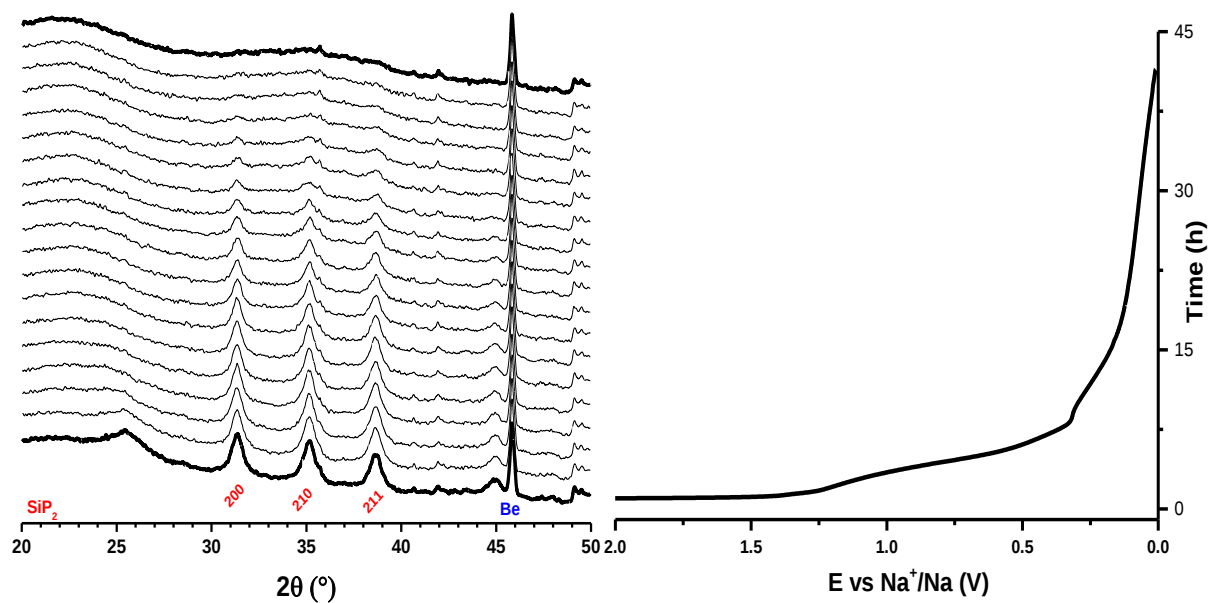


Figure S8 : Operando XRD of SiP_2/Na .

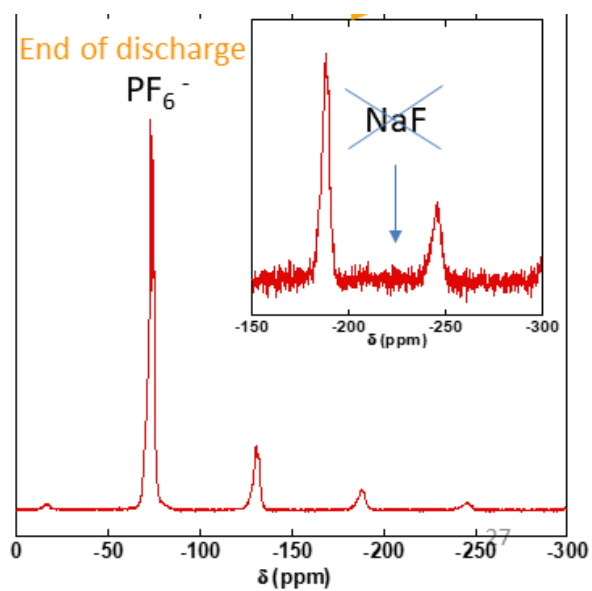


Figure S9: ^{19}F MAS NMR spectra for SiP_2 electrode stopped at the end of discharge.

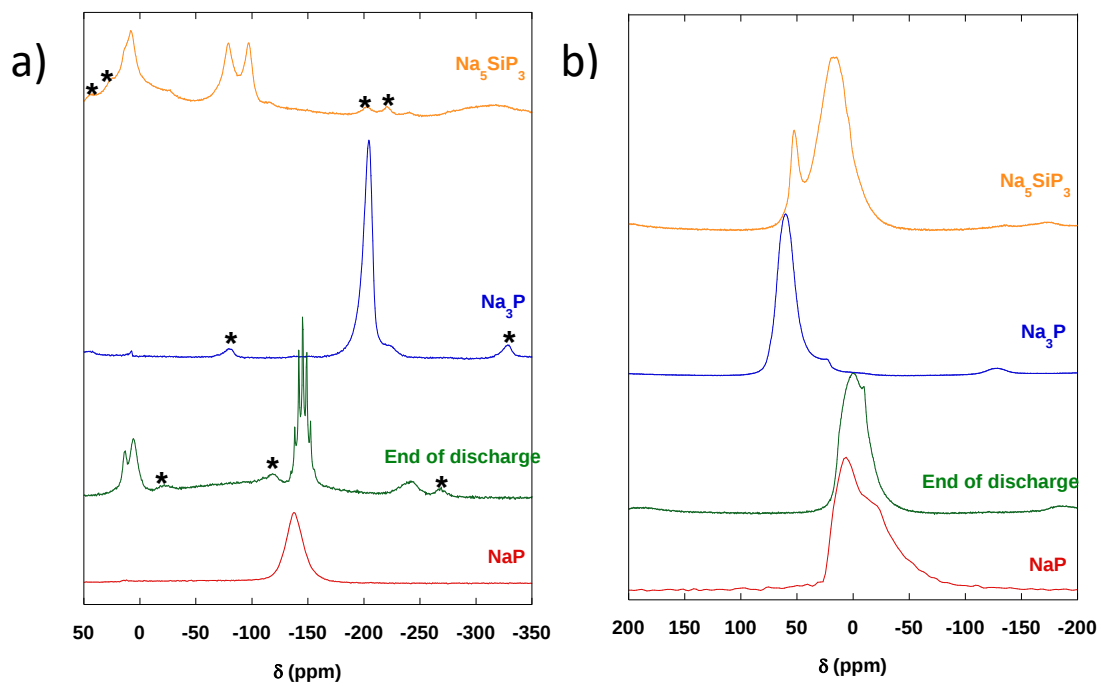


Figure S10: a) ^{31}P and b) ^{23}Na (right) MAS NMR spectra for Na_5SiP_3 , NaP, Na_3P and a SiP_2 electrode stopped at the end of discharge.