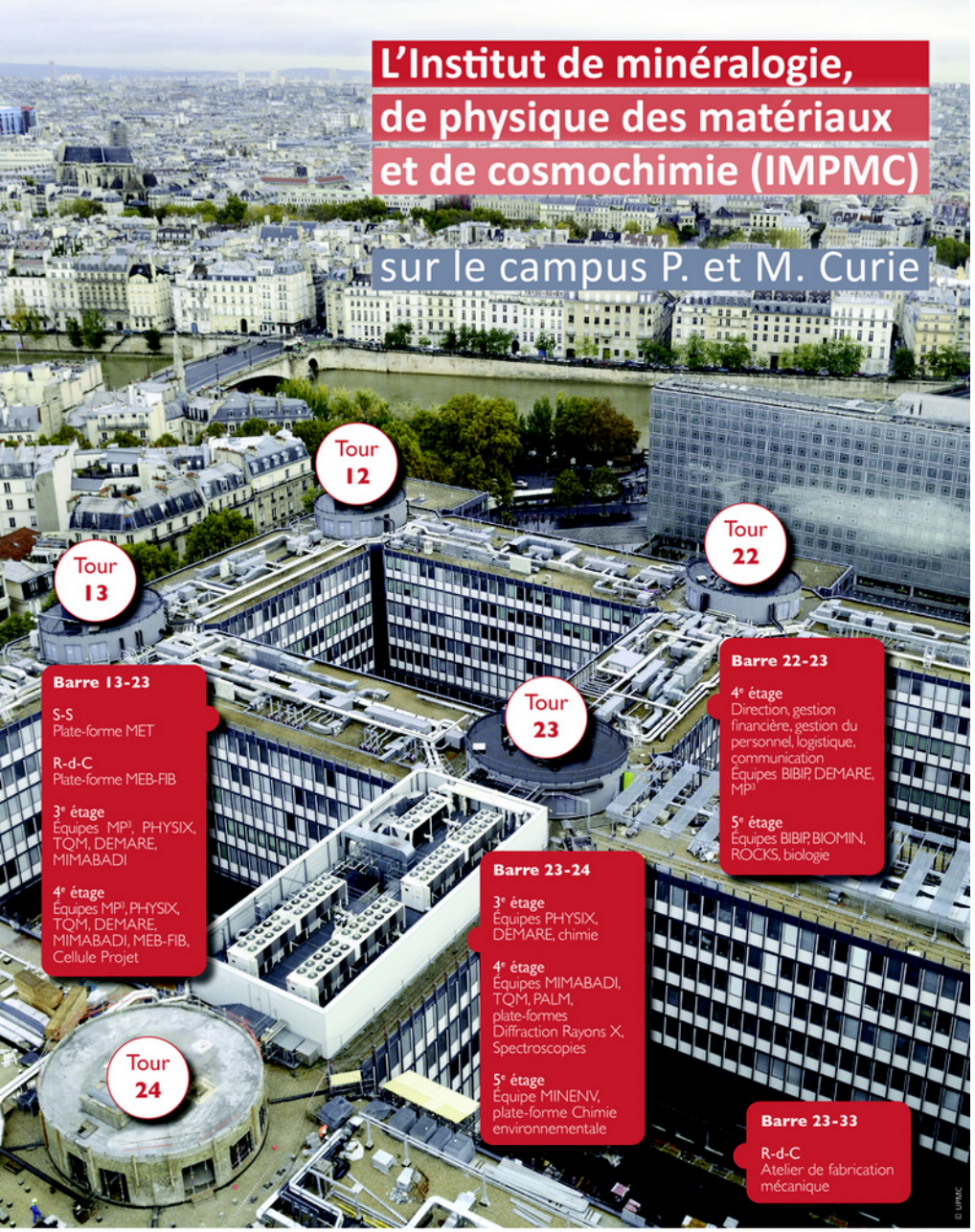
Institut de minéralogie,
de physique des matériaux
et de cosmochimie (IMPMC)

19/05/2021 – Lorenzo Paulatto

GdR
Nanomaterials For Energy Applications



UMR 7590 - Sorbonne Université/CNRS/MNHN/IRD

- Situated in the Jussieu campus in Paris 5e arrondissement
- About 80 research and teacher, 40 technical staff, 80 graduate students
- Director Marco Saitta
- Four *tutelles : Sorbonne Université, CNRS, Muséum National d'Histoire Naturelle, Institut de Recherche pour le Developpement*

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- Mineralogy and magnetism at low dimensionality
- Quantum theory of matter
- Physics of simple systems under extreme conditions
- Design and study of novel materials with remarkable electronic properties
- Properties of amorphous, liquids and minerals
- Mineralogy, Petrology and Planetary Physics
- Environmental mineralogy
- Cosmochemistry
- Research on Carbon-rich Key Samples
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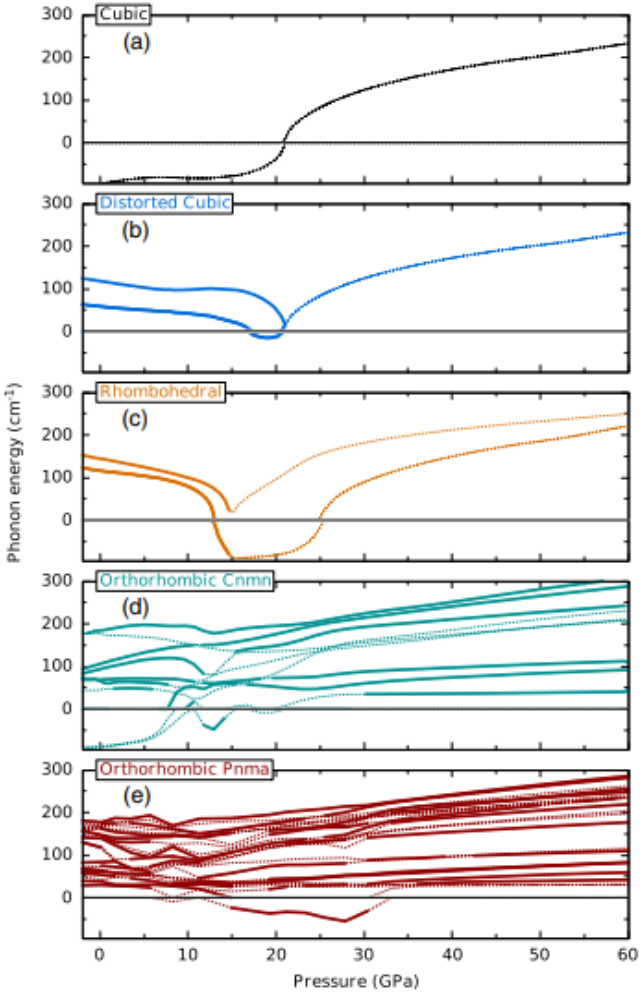
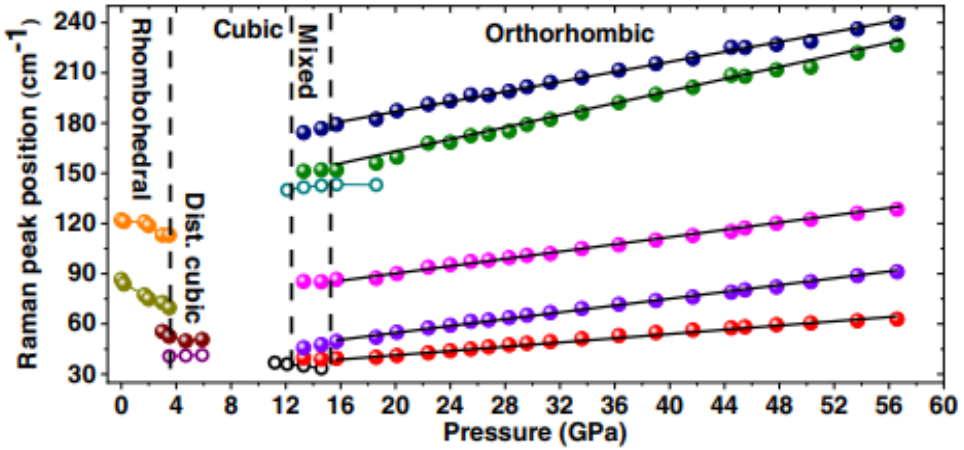
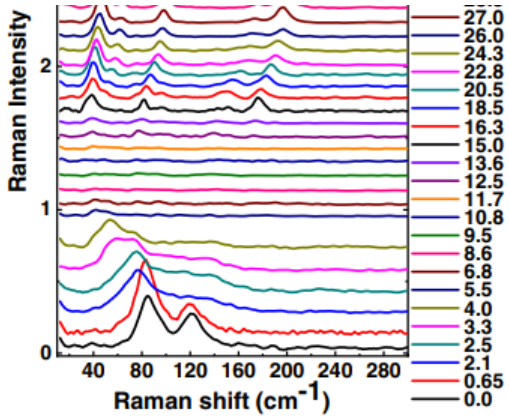
Characterization of chalcogenides





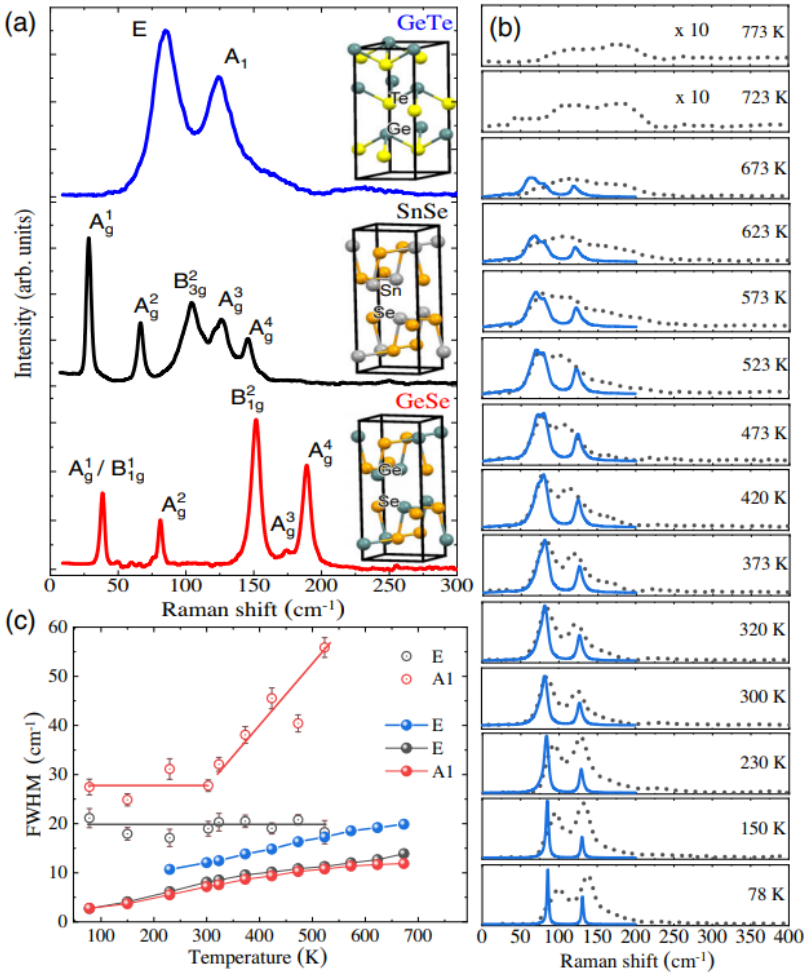


PHYSICAL REVIEW LETTERS **122,** 145701 (2019)

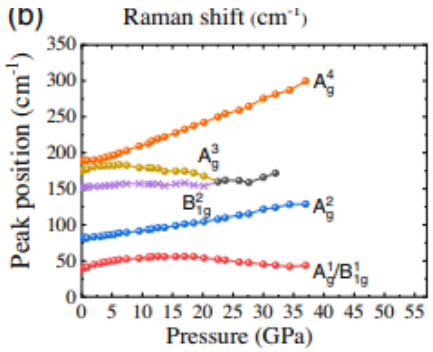
Pressure-Induced Phase Transitions in Germanium Telluride: Raman Signatures of Anharmonicity and Oxidation

Amit Pawbake,[1,*] Christophe Bellin,[1] Lorenzo Paulatto,[1] Keevin Béneut,[1] Johan Biscaras,[1] Chandrabhas Narayana,[2] Dattatray J. Late,[3] and Abhay Shukla[1,†]

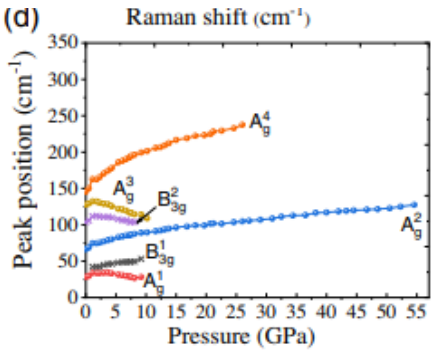
Characterization of chalcogenides



SnSe



GeSe



PHYSICAL REVIEW LETTERS **125,** 145301 (2020)

Functional Monochalcogenides: Raman Evidence Linking Properties, Structure, and Metavalent Bonding

Christophe Bellin,[1,*] Amit Pawbake,[1,2,*] Lorenzo Paulatto,[1] Keevin Béneut,[1] Johan Biscaras,[1] Chandrabhas Narayana,[3] Alain Polian,[1] Dattatray J. Late,[4] and Abhay Shukla[1,†]

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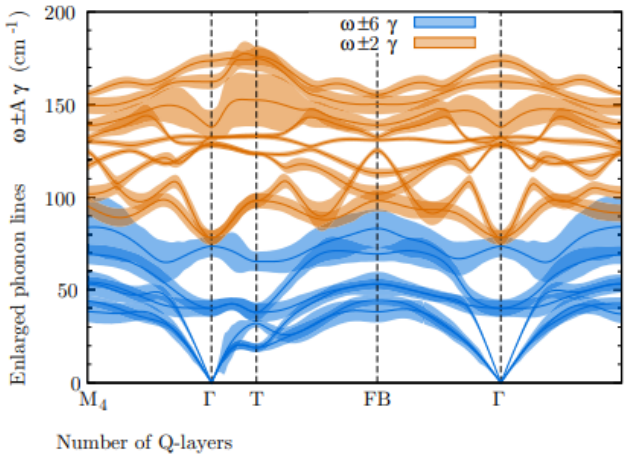
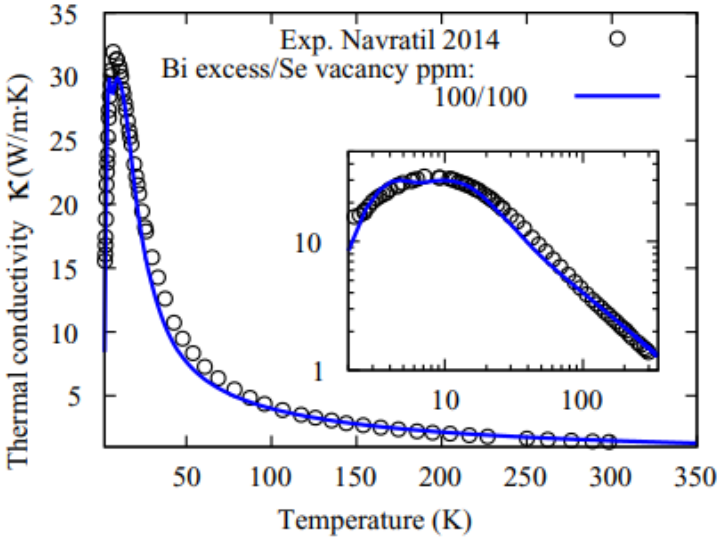
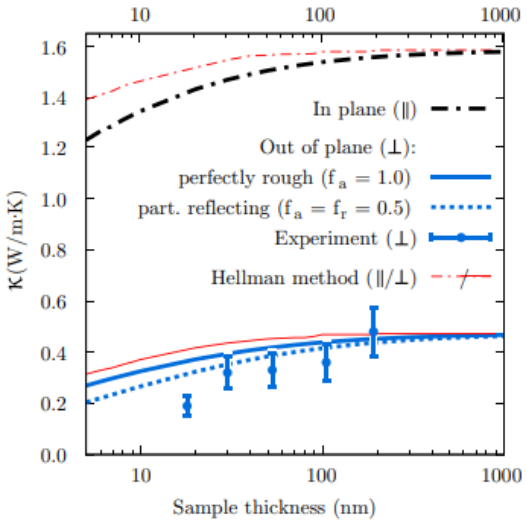
Thermal transport in nano-structured Bi_2Se_3

Ab-initio modelling of thermal transport including dfpt anharmonicity, impurities, intercalation and finite size effects.







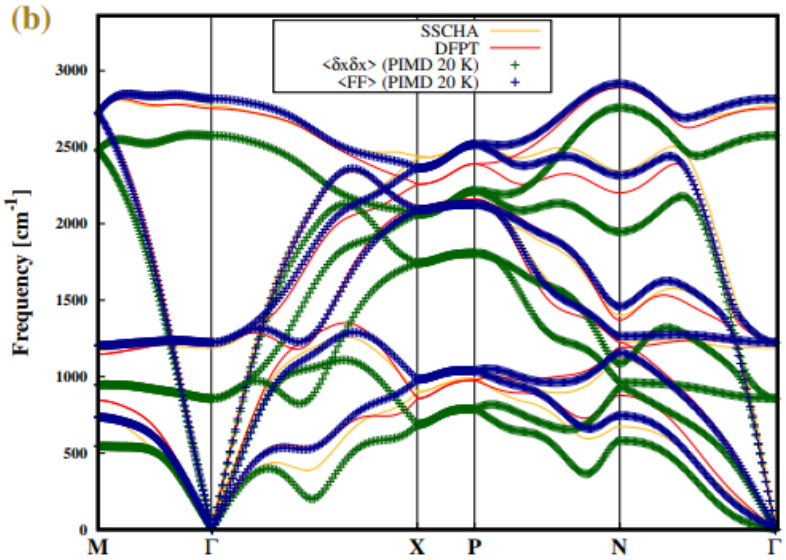
PHYSICAL REVIEW B **101**, 205419 (2020)

Thermal conductivity of Bi_2Se_3 from bulk to thin films: Theory and experiment

Lorenzo Paulatto*
Sorbonne Université, CNRS, Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, IMPMC, UMR 7590, 4 place Jussieu, 75252 Paris Cedex 05, France

Danièle Fournier, Massimiliano Marangolo, Mahmoud Eddrief, Paola Atkinson, and Matteo Calandra
Sorbonne Université, CNRS, Institut des NanoSciences de Paris, INSP, UMR 7588, F-75005 Paris, France

Simulation of strongly anharmonic materials



How to obtain phonons from path-integral molecular dynamics that include quantum behaviour of ions

Autocorrelation of
Velocity / Force

Phonons as superposition of
Classical / Quantum
harmonic oscillators

T. Morresi, LP, M. Casula, R. Vuillemin

arXiv:2103.04094v2 [cond-mat.mtrl-sci] 17 Mar 2021

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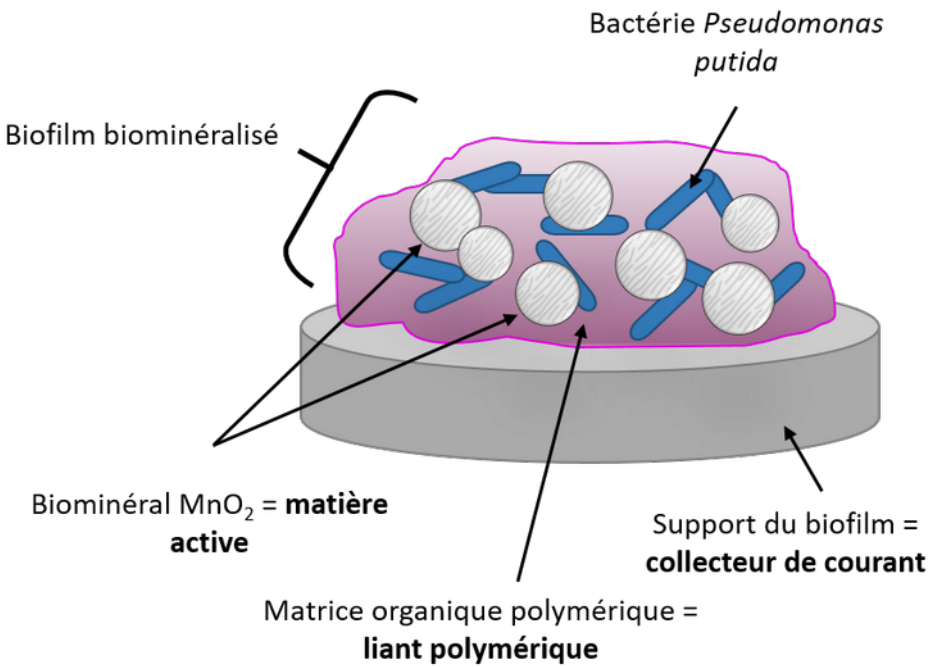
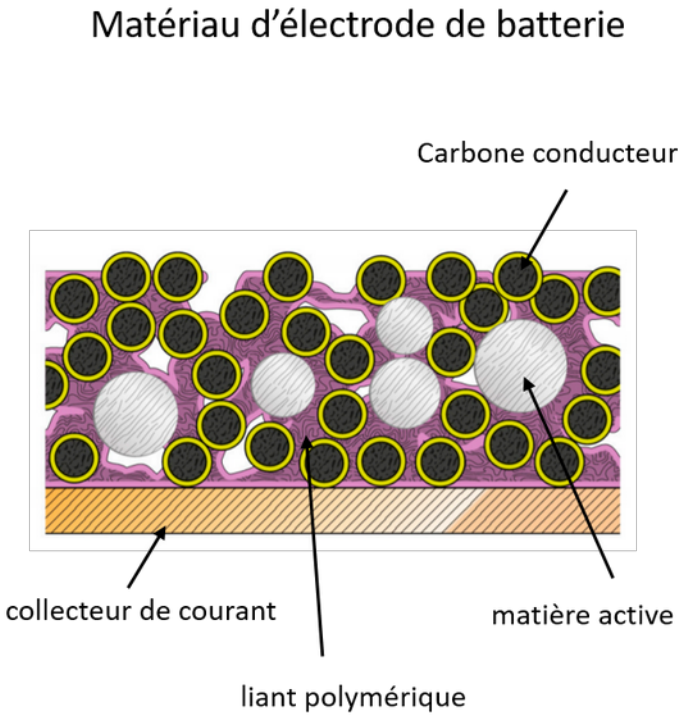
Formation of manganese oxides in biomineralized biofilm for electrochemical energy storage

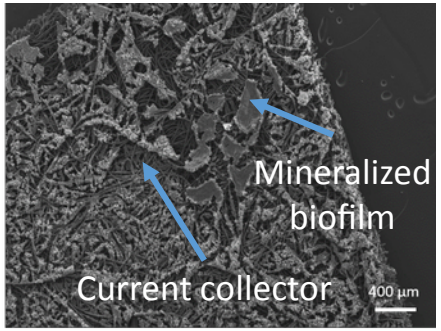
- Biomineralization of MnO_2 in **biofilm**
  - Control of biomaterial texture at electrode scale
  - One-pot production of Li-ion battery electrode material

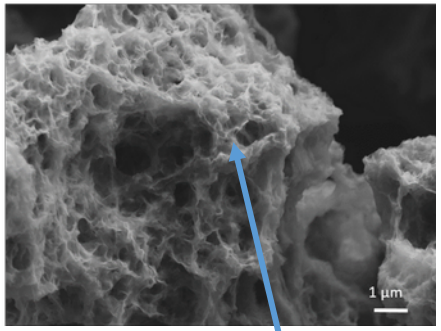




Formation of manganese oxides in biomineralized biofilm for electrochemical energy storage

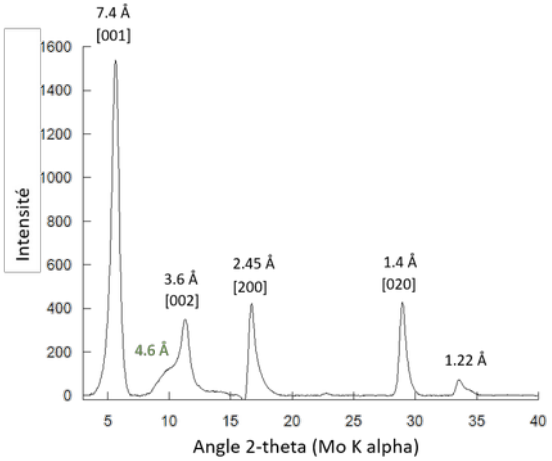
Single-step electrode production



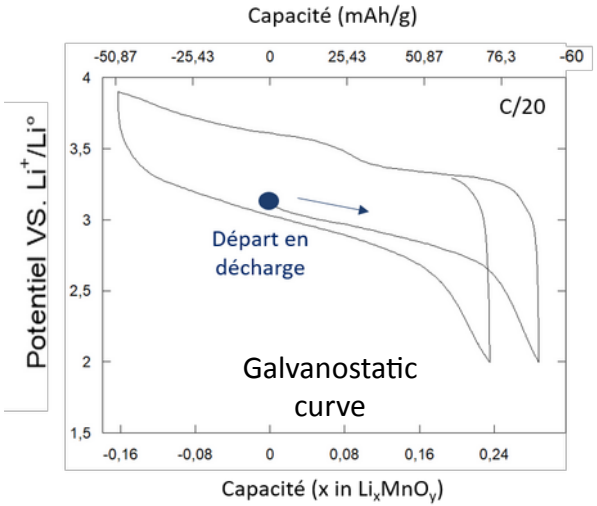


Mn oxyde in biofilm

Minerals:birnessite, layered Mn oxyde



Electro-chemical activity of single-step electrode from mineralized biofilm



Formation of manganese oxides in biomineralized biofilm for electrochemical energy storage

ORIGINAL RESEARCH ARTICLE

Front. Microbiol., 10 September 2020 | https://doi.org/10.3389/fmicb.2020.02031

Microbially Induced Mineralization of Layered Mn Oxides Electroactive in Li Batteries

Laura Galezowski[1], Nadir Recham[2,3], Dominique Larcher[2,3], Jennyfer Miot[1], Fériel Skouri-Panet[1] and François Guyot[1,4*]

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