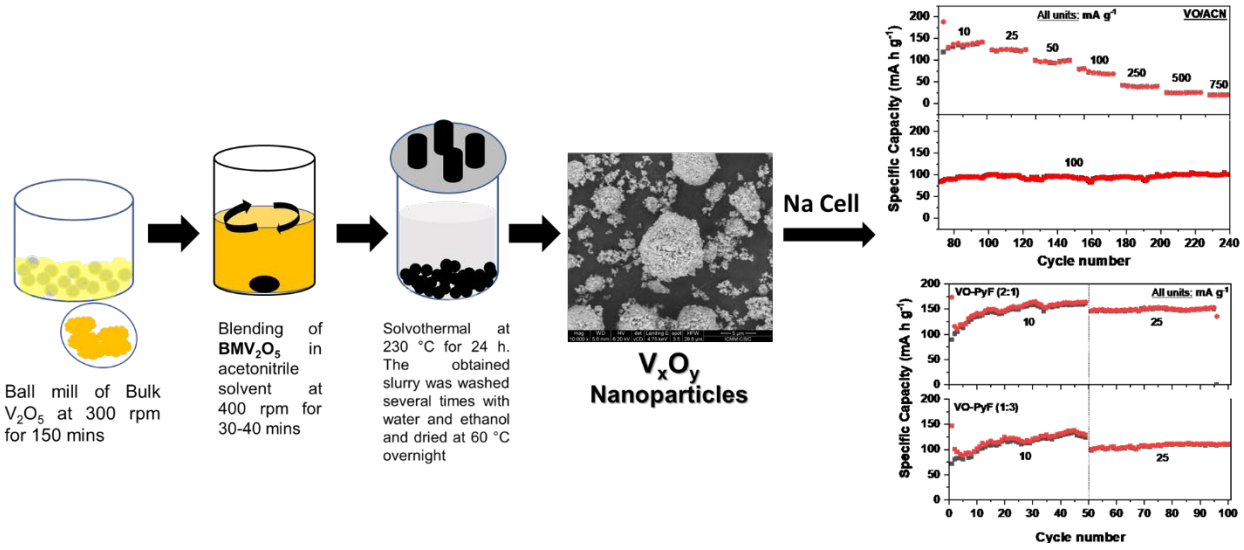
TITLE: Designing of Novel Mixed Anion Compounds as High Voltage and High Energy Density Sodium-ion Battery Cathodes (Grant Agreement 898624)

Summary of the project

Sodium-ion batteries (SIBs) are being developed and explored as potential electric storage for the grid applications due to infinite resources for sodium at cheaper price. The major impediment for its commercialization is unavailability of cathodes that possesses high output voltage and delivers high energy density. The state-of-art SIB positive electrodes consist of cathodes with the highest output potential (≤ 3.5 V) exhibiting lower specific capacities (150 mA h g^{-1}) while V_2O_5 cathodes delivered high specific capacity (225 mA h g^{-1}) at low potential (2.5 V). Therefore, it will be beneficial to design cathodes with high output voltage and capacity to build high energy density SIBs. In this project, the above drawbacks are mitigated by designing a new class of mixed anion compounds, vanadium oxyfluorides as novel cathode materials which are expected to deliver high specific capacities at higher operating voltage (≥ 3 V). These compounds are synthesized by partial fluorination using a non-hazardous organic reagents and novel one-pot solvothermal methods. The as-prepared materials were electrochemically tested as positive electrodes in a typical CR2032 half-cell coin cells against sodium between 1.0 – 3.5 V at specific current densities (mA g^{-1}).



The above scheme shows a glimpse of the material synthesis, physical, and electrochemical characterizations of the materials. The synthesized materials consisted of V_xO_y nanoparticles with: (1) enhanced inter-layer spacing due to intercalation of nitrile group between V_2O_5 layers which exhibited a specific capacity of ~100 mA h g^{-1} at 100 mA g^{-1} for > 150 cycles (VO-ACN); (2) secondly, fluorination of (large inter-layer spaced) V_xO_y using organic chemicals (such as Pyfluor); (3) Fluorinated V_xO_y exhibited ~150 and ~160 mA h g^{-1}, respectively, at 10 and 25 mA g^{-1} for each 50 cycles as sodium cathodes. However, structural and phase determination of these nanomaterials are in process using powder XRD, GIXRD and HRTEM techniques.

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Publications

1. **Chandrasekar M Subramaniyam**, Alois Kuhn, Isabel Barroso-Martín, Flaviano García-Alvarado, Enrique Rodríguez Castellón, "*Facile One-Pot Transformation of 0D V_2O_5 Nanoparticulates to 2D V_2O_3 Nanosheets For Superior Lithium and Sodium Storing Anodes*" (under preparation)
2. Structural determination of ball-milled V_2O_5-ACN as sodium cathodes (under analysis and manuscript preparation)
3. Fluorination of ball-milled V_2O_5 using Select- and/- Py-Fluors as sodium cathodes (under analysis and manuscript preparation)
4. Novel synthetic approach to innovative oxyfluorides (under analysis and manuscript preparation)

Public engagement activities

Outreach activities:

- European Researcher's Night (2021)
- Semana de la ciencia y la innovación: Una ciencia para los grandes retos de la humanidad (2021)
- European Researcher's Night (2022)

University website News:

- https://www.uspceu.com/en/press-room/new/marie-curie-researcher-sodium-batteries

Other activities

Research visits / secondments:

1) 2 months secondment at ICMM-CSIC (February 1, 2022 – March 31, 2022) performing 19F and 23Na MAS-NMR spectroscopy at different temperatures, analyzing the local structure (possible short range O2-/F- ordering) and mobility of sodium in previously synthetized vanadates and intercalated phases.
2) 3 months secondment at Universidad de Málaga (October 1, 2022 – December 22, 2022) performing XPS studies on vanadium oxides based sodium cathodes.

Teaching activities:

Taught 'General Chemistry' for 1st year under-graduate students (November – December 2021).

Supervision of students:

General technical discussion with PhD students in the research group.