Selectivity Mechanism of Cobalt Precipitation by an Imidazole Linker From an Old Battery Solution

Authors : Anna-Caroline Lavergne-Bril, Jean-François Colin, David Peralta, Pascale Maldivi

Abstract : Cobalt is a critical material, widely used in Li-ion batteries. Due to the planned electrification of European vehicles, cobalt needs are expending – and resources are limited. To meet the needs in cobalt to come, it is necessary to develop new efficient ways to recycle cobalt. One of the biggest sources comes from old electrical vehicles batteries (batteries sold in 2019: 500 000 tons of waste to be). A closed loop process of cobalt recycling has been developed and this presentation aims to present the selectivity mechanism of cobalt over manganese and nickel in solution. Cobalt precipitation as a ZIF material (Zeolitic Imidazolate framework) from a starting solution composed of equimolar nickel, manganese and cobalt is studied. A 2-MeIm (2-methylimidazole) linker is introduced in a multimetallic Ni, Mn, Co solution and the resulting ZIF-67 is 100% pure Co among its metallic centers. Selectivity of Co over Ni is experimentally studied and DFT modelisation calculation are conducted to understand the geometry of ligand-metal-solvent complexes in solution. Selectivity of Co over Mn is experimentally studied, and DFT modelisation calcucation are conducted to understand the link between pKa of the ligand and precipitration of Mn impurities within the final material. Those calculation open the way to other ligand being used in the same process, with more efficiency. Experimental material are synthetized from bimetallic (Ni^{2+}/Co^{2+}, Mn^{2+}/Co^{2+}, Mn^{2+}/Ni^{2+}) solutions. Their crystallographic structure is analysed by XRD diffraction (Brüker AXS D8 diffractometer, Cu anticathode). Morphology is studied by scanning electron microscopy, using a LEO 1530 FE-SEM microscope. The chemical analysis is performed by using ICP-OES (Agilent Technologies 700 series ICP-OES). Modelisation calculation are DFT calculation (density functional theory), using B3LYP, conducted with Orca 4.2.

Keywords : MOFs, ZIFs, recycling, closed-loop, cobalt, li-ion batteries

Conference Title : ICRMCEA 2023 : International Conference on Recyclable Materials in Civil Engineering Applications
Conference Location : Bangkok, Thailand
Conference Dates : January 16-17, 2023