Supplementary Information

Synthesis and Characterization of $LiCoO_2$ from Different Precursors by Sol-Gel Method

Bruno G. A. Freitas,[a] José M. Siqueira Jr.,*[a] Leonardo M. da Costa,[a] Glaucio B. Ferreira[a] and Jackson A. L. C. Resende[a,b]

[a]PPG em Química, Instituto de Química, Universidade Federal Fluminense, Outeiro de São João Batista, s/n, Campus do Valonguinho, Centro, 24020-141 Niterói-RJ, Brazil

[b]PPG em Ciências dos Materiais, Instituto de Ciências Exatas e da Terra, Universidade Federal do Mato Grosso, Centro Universitário do Araguaia, Avenida Universitária, 3500, 78698-000 Pontal do Araguaia-MT, Brazil

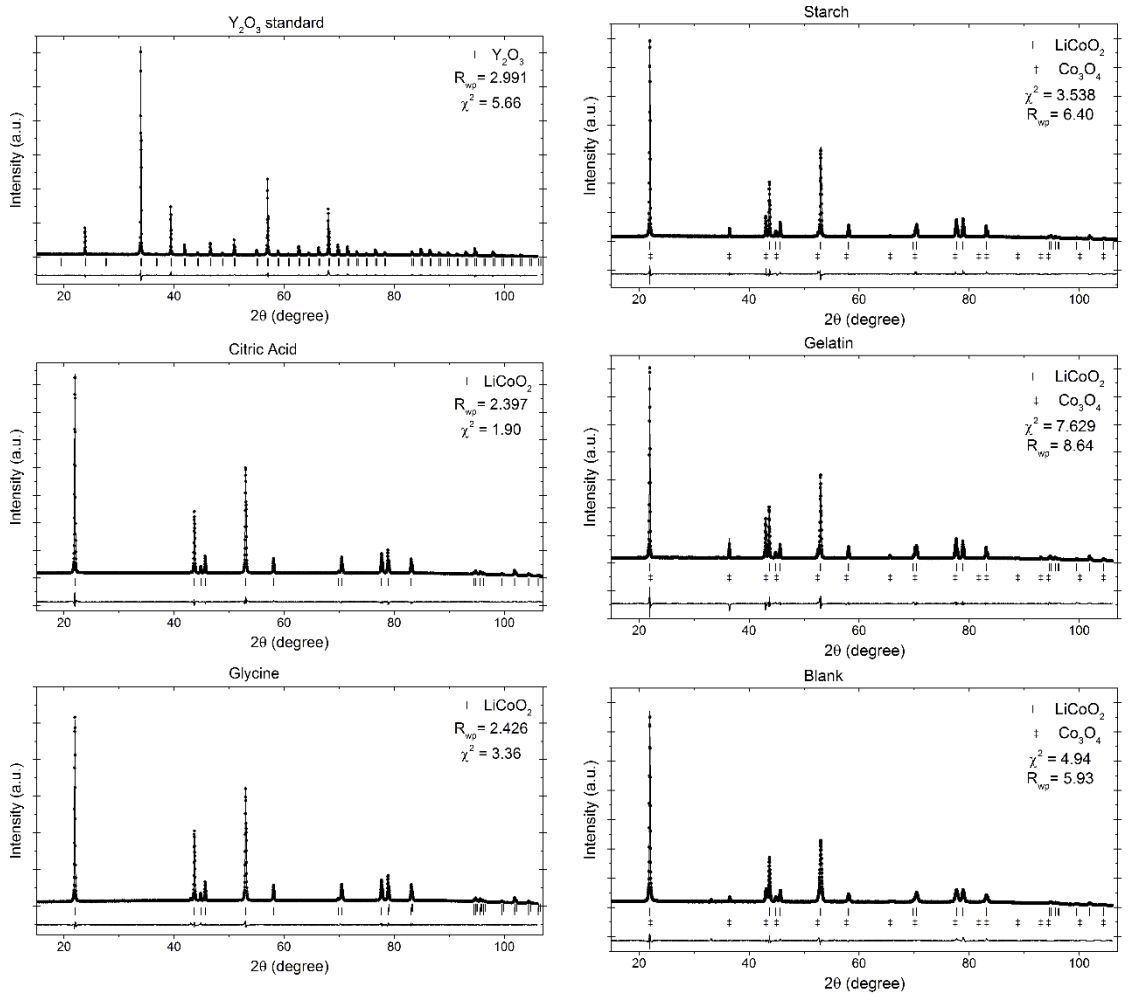

Figure S1. Rietveld refinement of XRD pattern of Y_2O_3 and of all samples studied. Performed with a Bruker D8 Advance, Co Kα radiation (λ 1.79026 Å), steps 0.02°, time of 0.5 s *per* step.

*e-mail: jmsiqueirajunior@id.uff.br

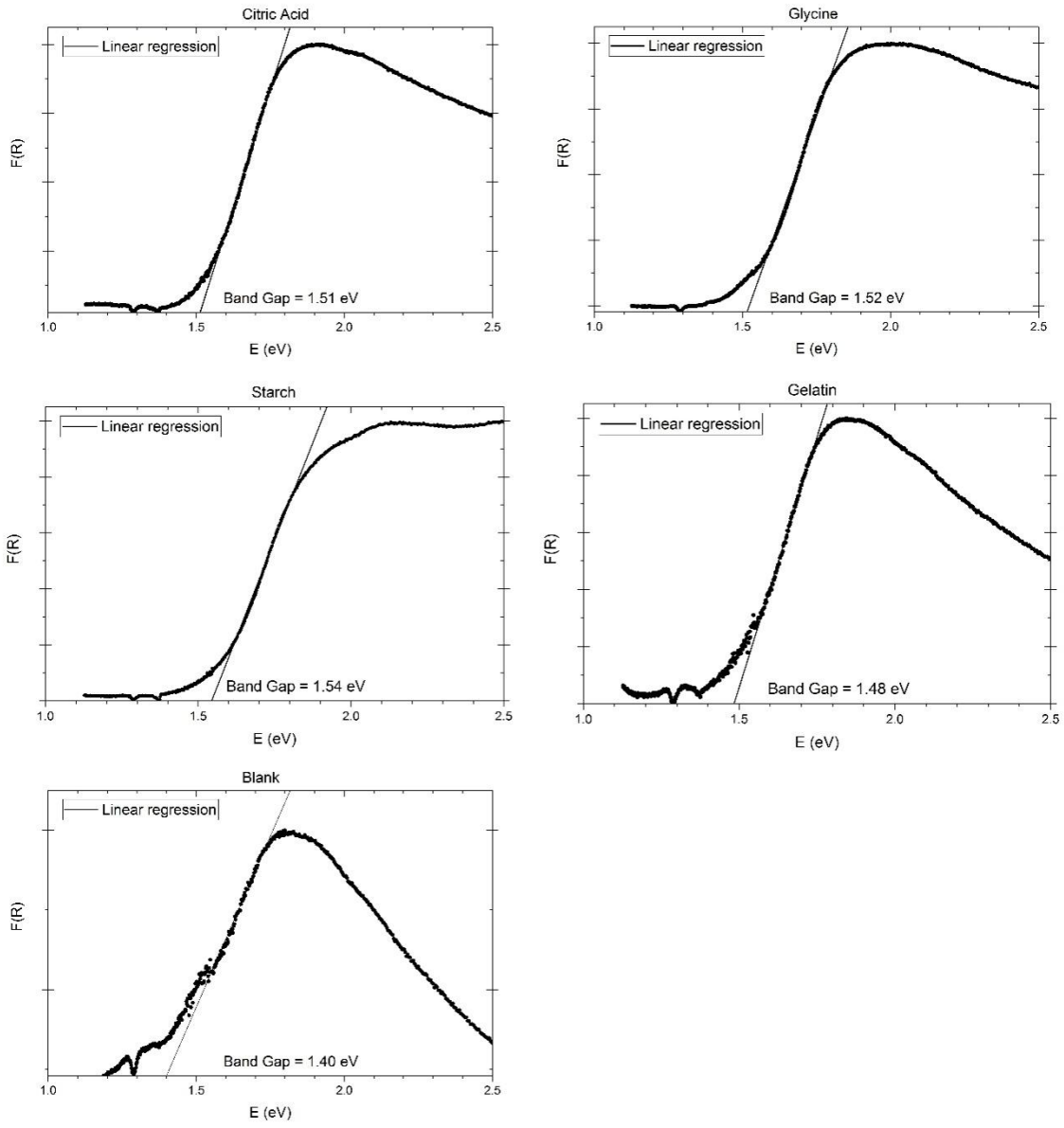

Figure S2. DRS, function Kubelka-Munk, F(R) and extrapolation of the tangent line for obtaining band-gap of all samples studied. Obtained in Cary 5000 Varian UV-Vis-NIR Spectrophotometer, wavelengths 190-950 nm, reference MgO.

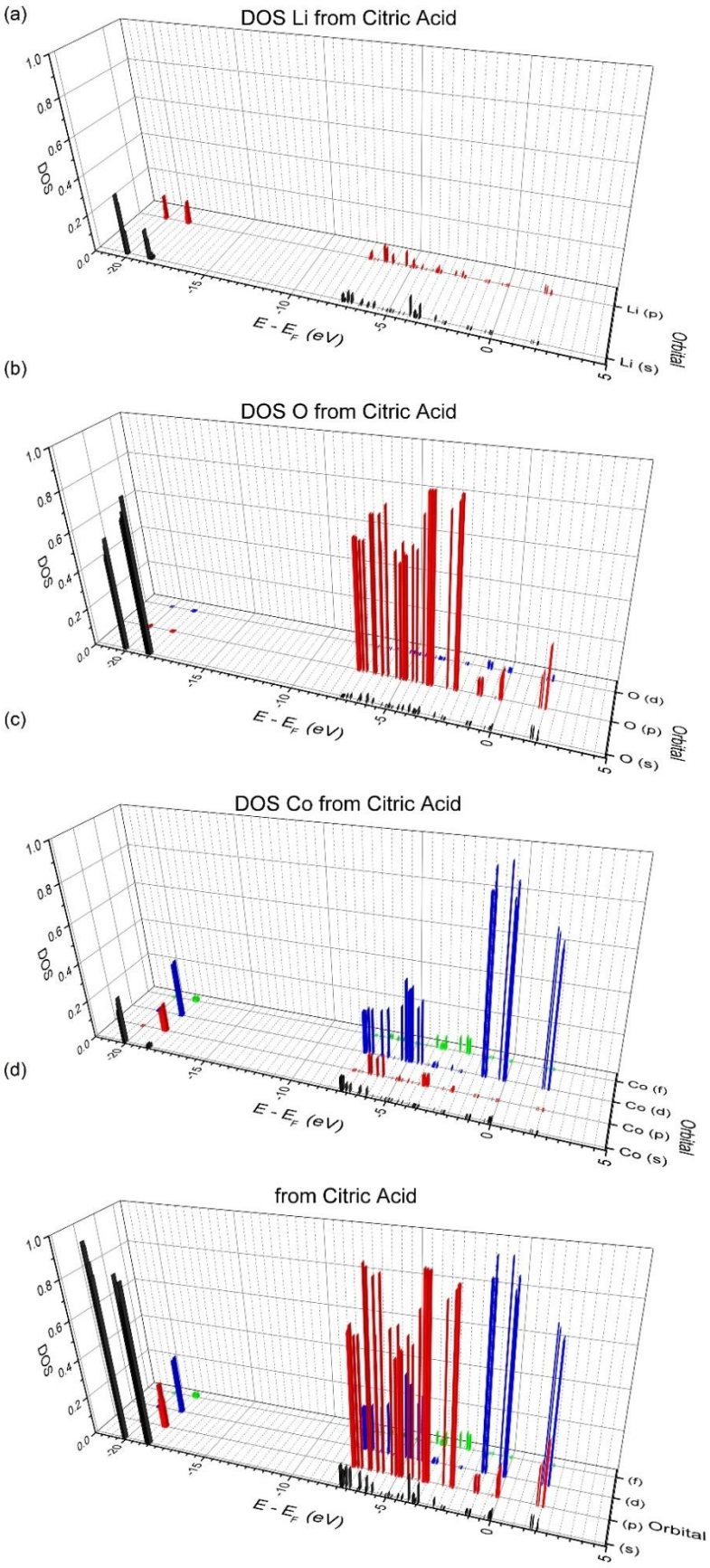

Figure S3. DOS for the $LiCoO_2$ in each orbital obtained from citric acid for each element and global. Method DFT/GGA, PBE functional, program CP2K, T (300K).

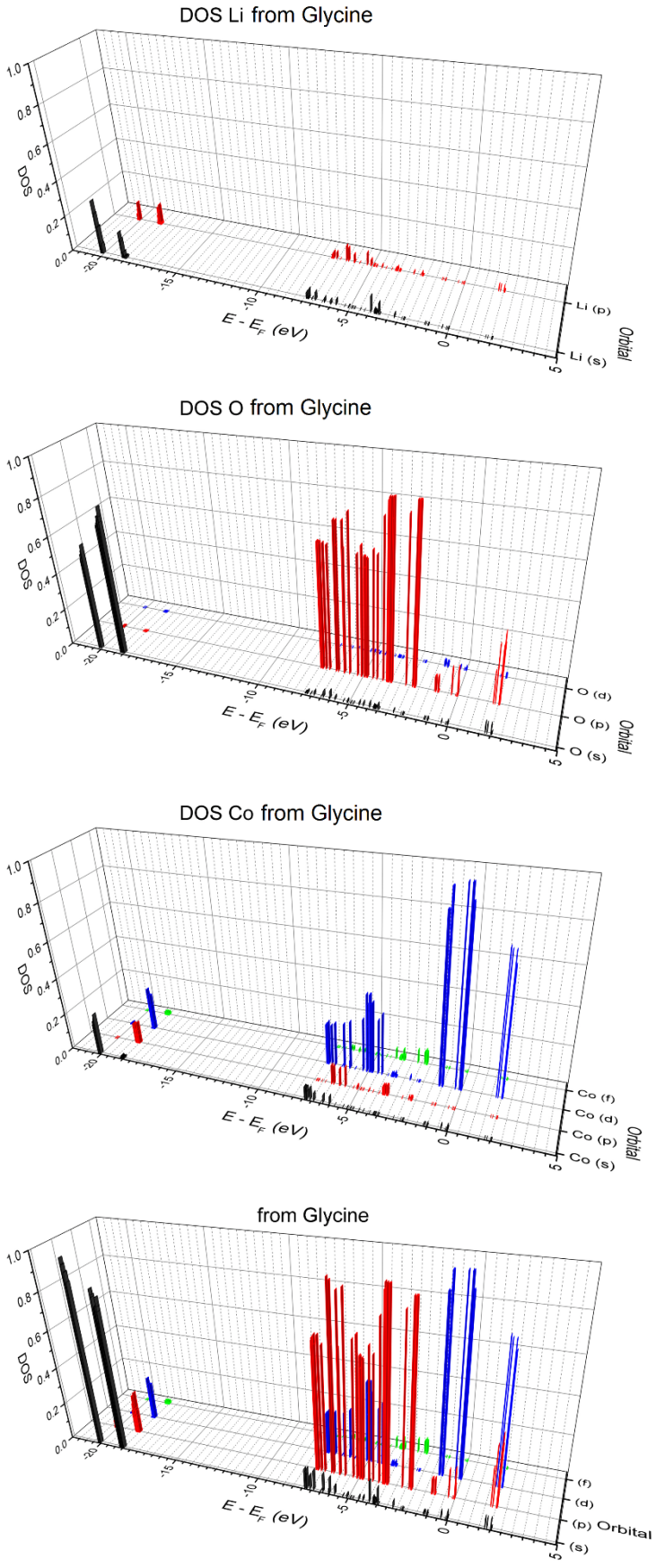

Figure S4. DOS for the $LiCoO_2$ in each orbital obtained from glycine for each element and global. Method DFT/GGA, PBE functional, program CP2K, T (300K).

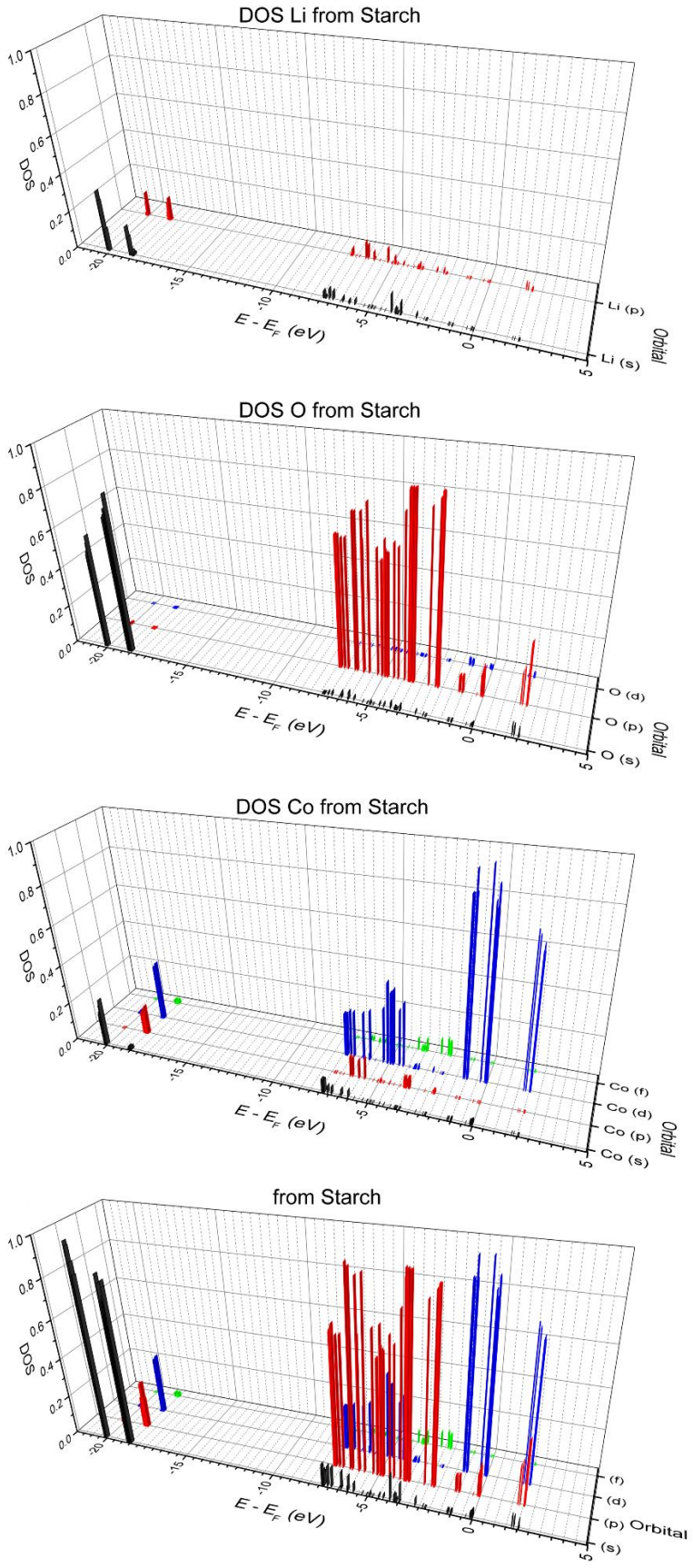

Figure S5. DOS for the $LiCoO_2$ in each orbital obtained from starch for each element and global. Method DFT/GGA, PBE functional, program CP2K, T (300K).

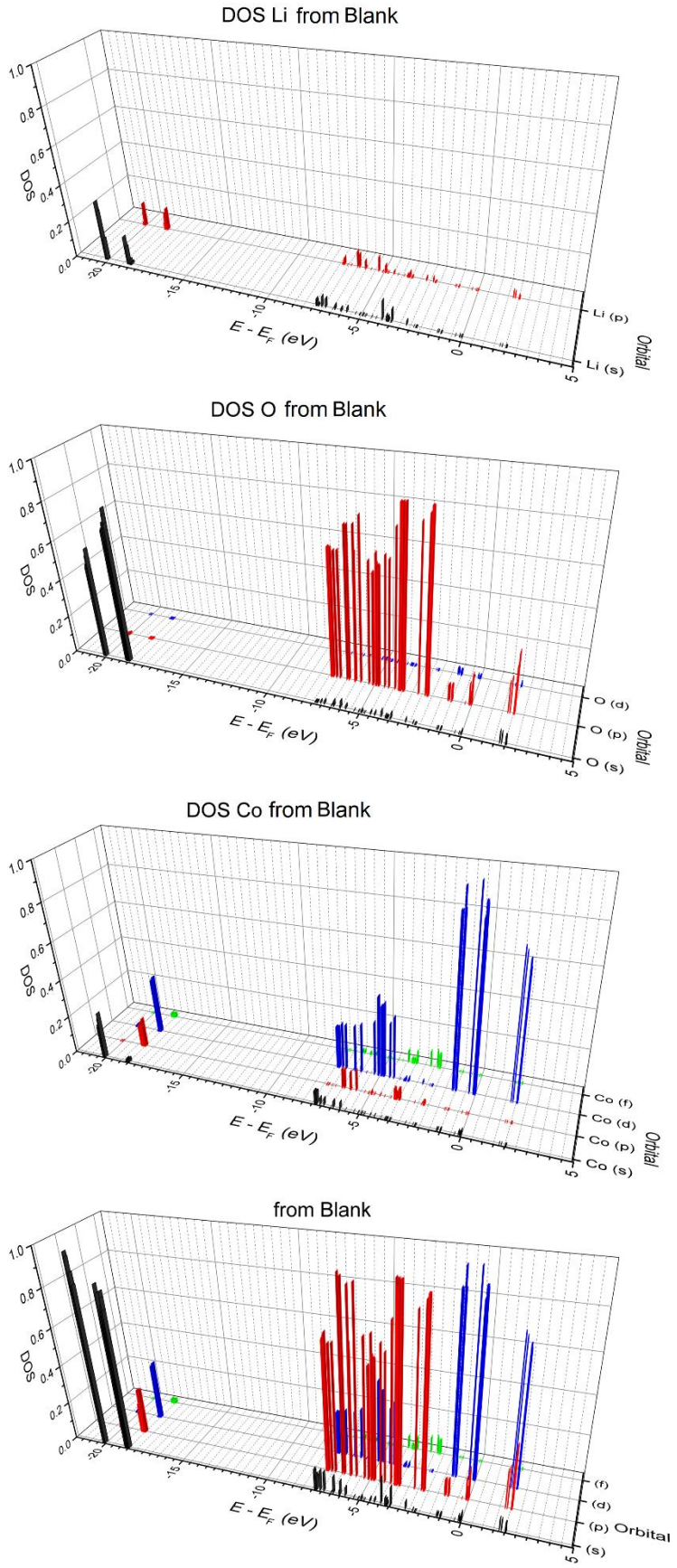

Figure S6. DOS for the $LiCoO_2$ in each orbital obtained from test blank for each element and global. Method DFT/GGA, PBE functional, program CP2K, T (300K).

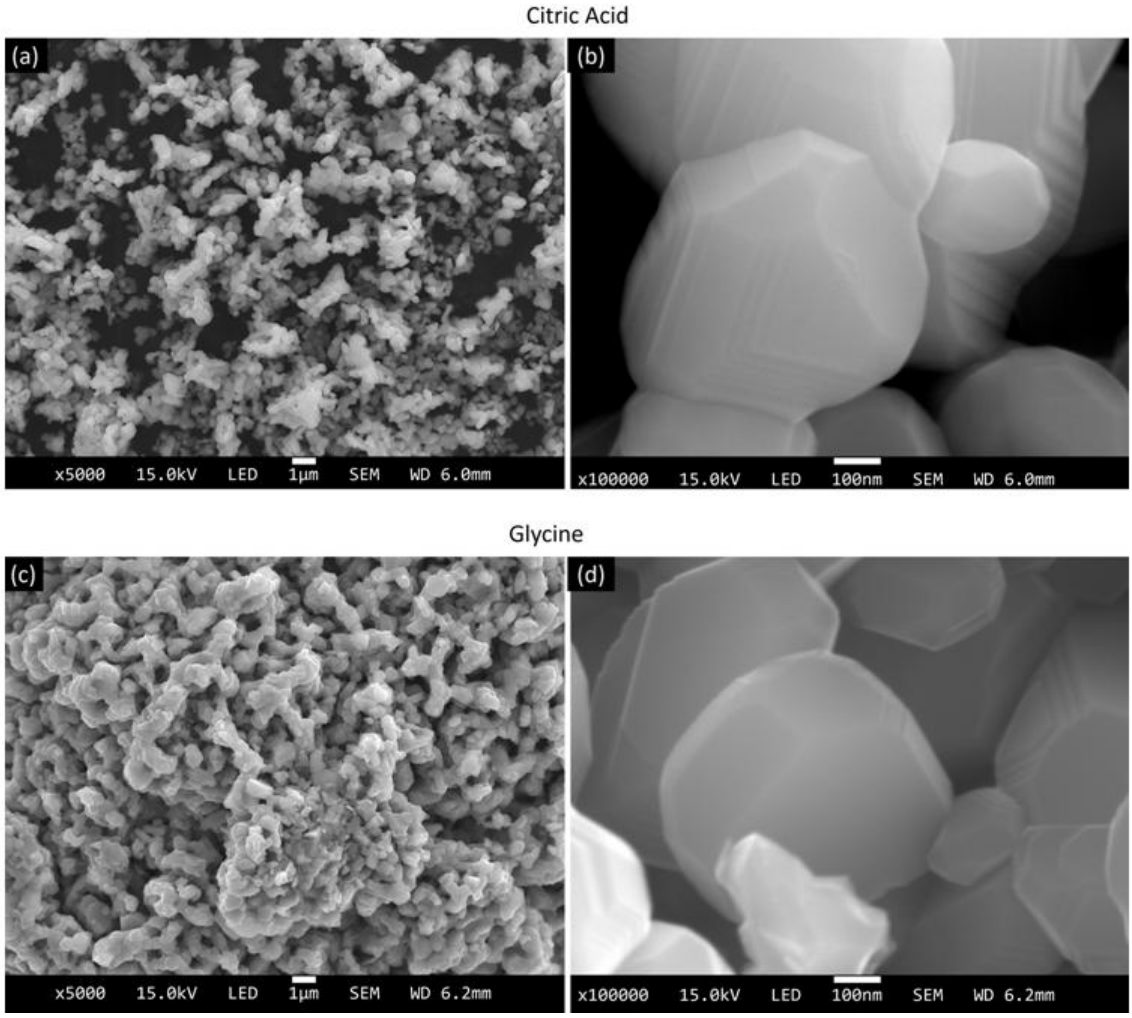

Figure S7. SEM of the synthesized samples by citric acid expanded (a) 5000×, (b) 100000×; and by glycine expanded (c) 5000× and (d) 100000×. Using JEOL JSM-7100F, voltage 15.0 kV, tape of carbon on a metal support.