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ABSTRACT:

Toward a Self-Driving Lab for the Development of Functional Oxides

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The quest for advanced functional oxides has been hindered by the time intensive nature of conventional research methods. Acceleration strategies include the combinatorial approach which accelereated research by parallelising the production and characterization of many compositions. Acceleration strategies also include self driving laboratories, in which materials are usually produced in a sequential manner but the composition space is potentially much wider and the composition is optimised in a fully automated way after the targte property definition. The self-driving laboratory combines cutting-edge robotics for automated synthesis and characterisation, coupled to machine learning and data analytics. We present here the implementation of the ExploraMat platform, a self-driving laboratory for functional oxide materials development. The development includes materials deposition from polymer-assisted deposition, whose preparation is made automatically starting from till 8 « mother » solutions, and thermal treatment of as-deposited layers. The automated deposition step includes visual controling to verify the suitability of the deposition parameters. The platform also foresees to include X-ray-diffraction and ellipsometry characterisation, whose characterisation are meaningfull in a self-driving lab only if an automated analysis approach is developed. We will see that both machine-learming and more classical approaches are able to deal with the automated characterisation challenges. Finally, we present some tools developed for the characterisation of functional properties, such as piezocatalysis or ion conduction.