Deep neural networks for the analysis of X-ray photoelectron spectroscopy data.

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In this work, we characterize the performance of a deep neural network designed to detect and quantify chemical elements in experimental X-ray photoelectron spectroscopy data. In order to train the neural network, we computed a large (100 k) dataset of synthetic spectra, based on randomly generated materials covered with a layer of adventitious carbon with random thickness. The trained net has been tested on about 500 well characterized X-ray spectra. Fine details about the net layout, the choice of the loss function and the quality assessment strategies are also discussed. Given the synthetic nature of the training set, this approach could be applied to help the automatization of any photoelectron spectroscopy system, without the need of experimental reference spectra and with a low computational effort.