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Computational XPS from Koopmans compliant Functionals NICOLAS POILVERT, NATHAN KEILBART, ISMAILA DABO, The Pennsylvania State University — X-Ray Photo-emission Spectroscopy (XPS) is one of the most accurate experimental probe when it comes to deciphering the **chemical composition** of materials like Transition-Metals and Transition-Metal Oxides. Because of the sensitivity of *electron binding energies* to the local chemistry surrounding an atom, XPS can also help identify atomic **oxidation states**. Nevertheless the complexity of XPS signals makes it a hard task to go from a spectra to a list of chemical species and their associated oxidation states. Electronic structure methods such as Density Functional Theory fall short when it comes to predicting electron binding energies because of large self-interaction errors. The recent introduction of Koopmans-compliant functionals[1,2] on the other hand has led to the conclusion that UPS spectra can be accurately predicted at the level of **Many-Body Perturbation Theory** and beyond, while retaining most of the conceptual and computational simplicity of DFT. In this talk, we will more particularly focus our attention on assessing the accuracy of predicted Transition-Metal XPS spectra.

[1]I. Dabo et al., **Phy. Rev. B** 82, 115121 (2010)
[2]I. Dabo et al., **Phys. Chem. Chem. Phys.**, 15, 685-695 (2013)

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