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X-ray core-hole spectroscopy from first principles: Theory and applications

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Abstract: In this talk I will first outline the single particle theory of X-ray absorption spectroscopy and its implementation in the XSpectra code. I will consider both the case of K and L_2,3 edges. I will then present several applications performed with Xspectra, either by me and my coworkers or by several groups in very different fields of condensed matter. Finally, I will outline possible future developments and collaboration with the Team in Lausanne.

References:
[1] Christos Gougoussis, Matteo Calandra, Ari P. Seitsonen, and Francesco Mauri Phys. Rev. B 80, 075102 (2009).
[2] C. Gougoussis, M. Calandra, A. Seitsonen, Ch. Brouder, A. Shukla, and F. Mauri, Phys. Rev. B 79, 045118 (2009).