Challenges in ELNES/NEXAFS: the handicap of current simulation

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EELS with its unquestionable high lateral resolution and XAS under real reaction conditions have made ELNES and NEXAFS become unique ways to evaluate the local electronic structure and identify the active phases in catalytic reactions. Recently, as monochromator and high stable tank are becoming more available, EELS with improved energy resolution gives access to the same information as the synchrotron. Recently, it was shown that vanadium L_3 ELNES and NEXAFS of V_2O_5 with identical spectral feature could be obtained by applying dedicated Philips 200 kV (S)TEM [1]. However, as it is shown in the figure, the calculated density of unoccupied state using WIEN97 code gives no way to interpret even one spectral feature [1]. Even calculation taking the core-hole effect into accout cannot satisfied results.

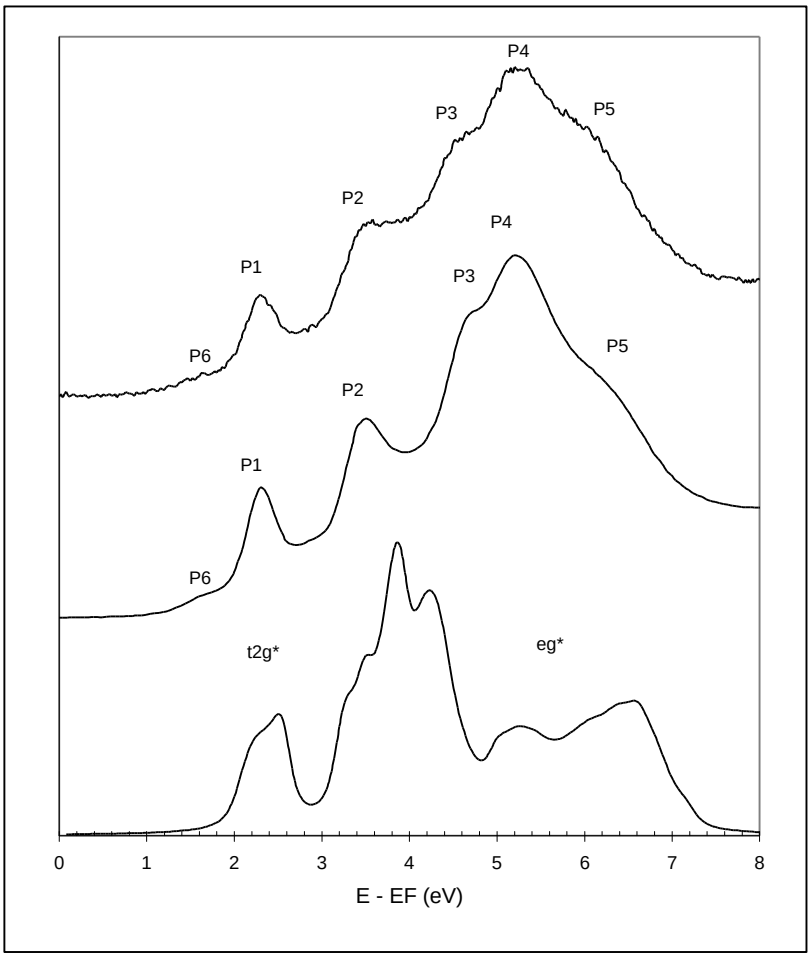

Figure 1: High-resolution V L_3 ELNES of V_2O_5 (top), compared with V L_3 NEXAFS (middle) and the simulated spectrum (bottom).

Recently, in-situ XAS has been applied to observe the dynamic structural surface rearrangements of vanadium phosphorus oxide catalysts [2]. Under the catalytic test condition, a temperature dependent dynamic behaviour of the V-L_3 NEXAFS was observed. Since no DOS of VPO is available, a tentative interpretation is given in term of specific V-O bonds in the VPO structure [2].

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Reference

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2. M. Hävecker, R.W. Mayer, A. Knop-Gericke, H. Bluhm, D.S.Su, J.A. Lopez-Sanchez, G.J. Hutchings, and R. Schlögl, submitted to J. Phys. Chem. B