

SUPPORTING INFORMATION

Investigation of the valence electronic states of Ti(IV) in Ti silicalite-1 coupling X-ray emission spectroscopy and density functional calculations

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In Figure S1, the spectra computed using TZVP/CP(PPP) basis sets and TPSSh density functional on the cluster T35_MFI are reported, changing the Ti position in the framework. As clearly visible from the figure no T-dependency was found. This is due to the local character of the technique.

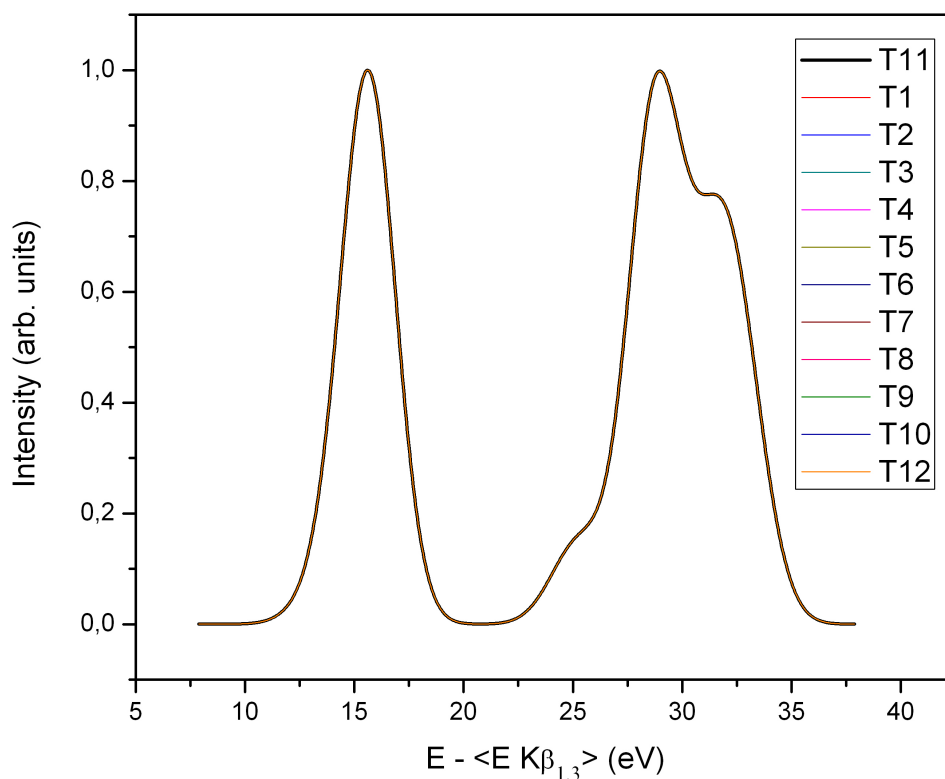


Figure S1: VtC-XES spectra computed adopting TPSSh/TZVP/CP(PPP) on the clusters T35_MFI, optimized with the Ti atom in one of the twelve non equivalent crystallographic positions.

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Table 1. Goodness factors for the VtC-XES spectra computed on the T5OH cluster using TZVP(ligands)/CP(PPP)(Ti) for a selection of density functionals.

Functional	ΔE_{\max} (eV)	ΔE_{cm} (eV)	I_C/I_B ratio (± 0.005)
LDA	17.7	17.9	0.829
GLYP	12.4	12.66	0.738
PBE	12.5	13.03	0.779
PWP	12.6	12.7	0.802
B1LYP	13.7	14.5	0.744
B3LYP	13.4	13.6	0.773
PBE0	13.8	14.1	0.79
TPSS	13.0	13.6	0.821
TPSSh	13.2	13.8	0.780
TPSS0	14.3	15.0	0.840
B2PLYP	15.2	16.1	0.823
Experiment	13.2	13.8	0.781