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Supporting Information

Infrared and X-Ray Photoelectron Spectroscopic Studies of the Reactions of Hydrogen-Terminated Crystalline Si(111) and Si(100) Surfaces with Br₂, I₂, and Ferrocenium in Alcohol Solvents

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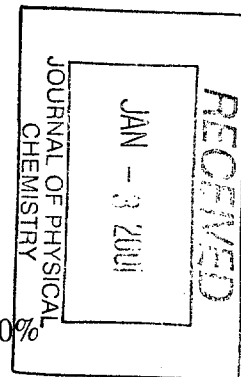


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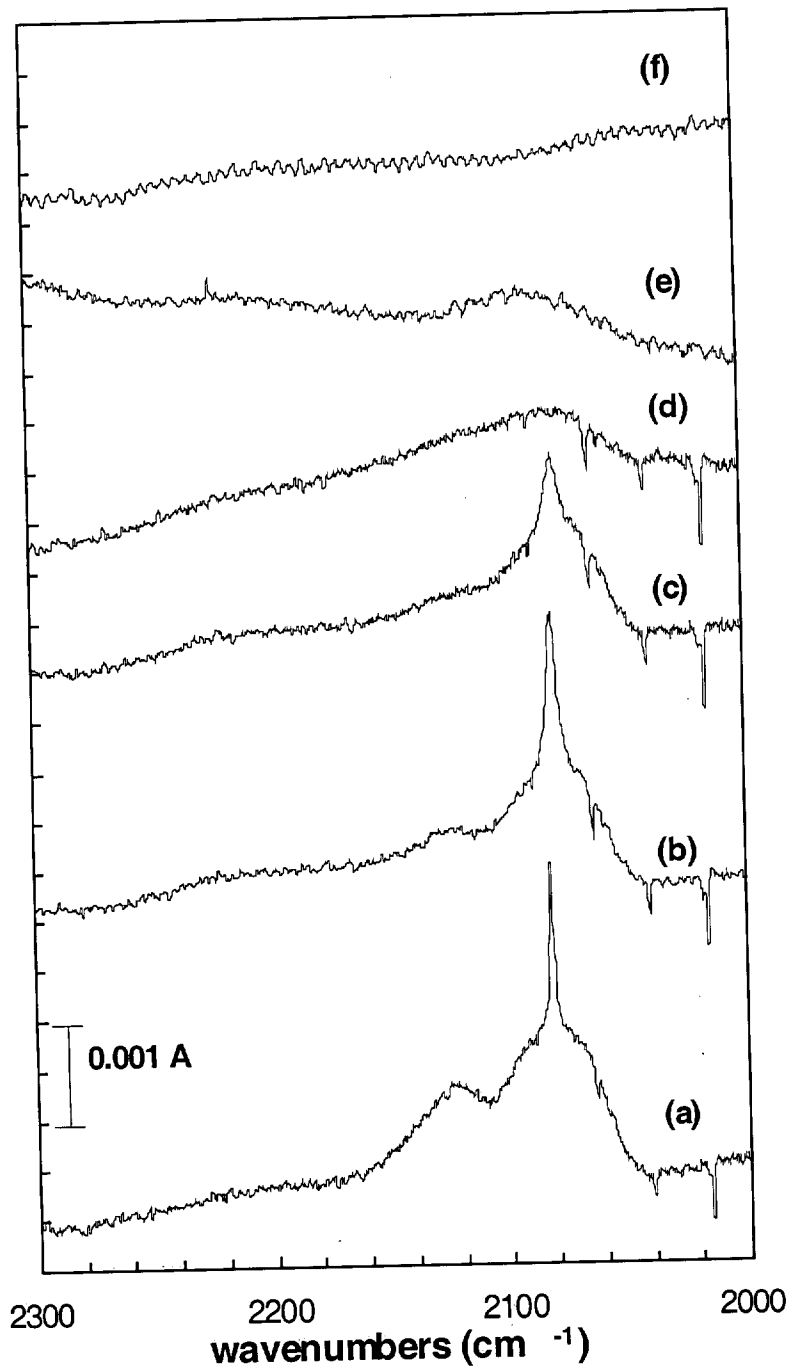


Figure 12. FT-IR spectra of a Si(111) ATR crystal after (a) etching in N_2 -sparged 40% $NH_4F(aq)$, (b) immersion for 5 min in CH_3OH , (c) immersion for 3-5 min in CH_3OH containing 200 mM ferrocene, (d) immersion for 3-5 min in CH_3OH containing 200 mM ferrocenium $[BF_4]$, (e) a different H-terminated ATR crystal after immersion for 15 min in CH_3OH containing 25 mM I_2 , (f) a different H-terminated ATR crystal after immersion for 15 min in CH_3OH containing 200 mM Br_2 . The data are the total absorbance produced by 50 reflections within the crystal.

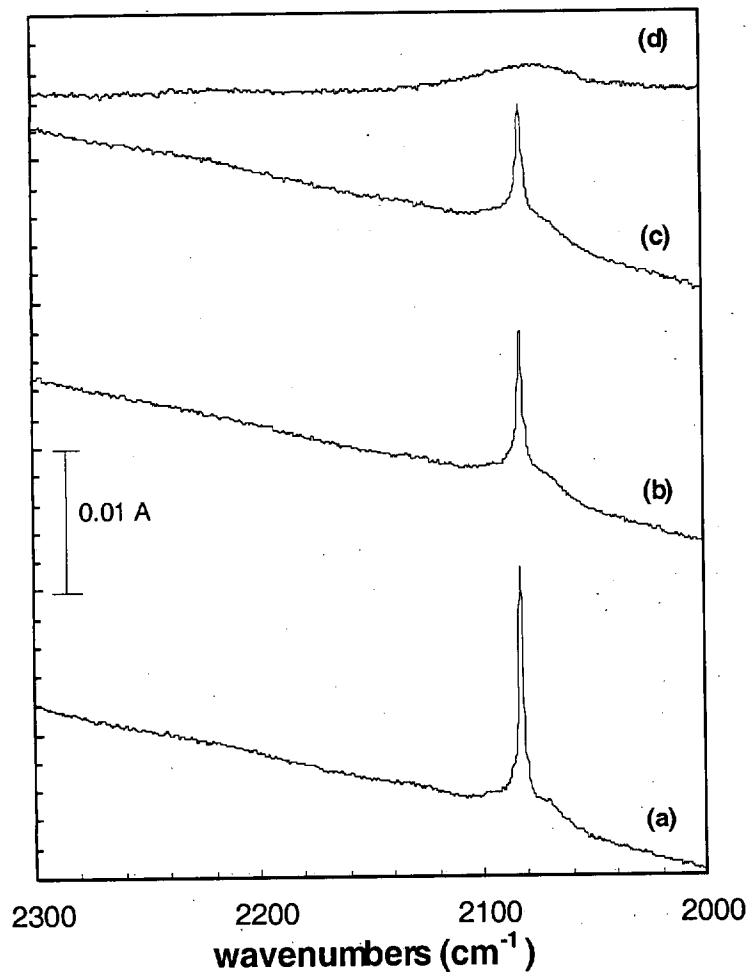


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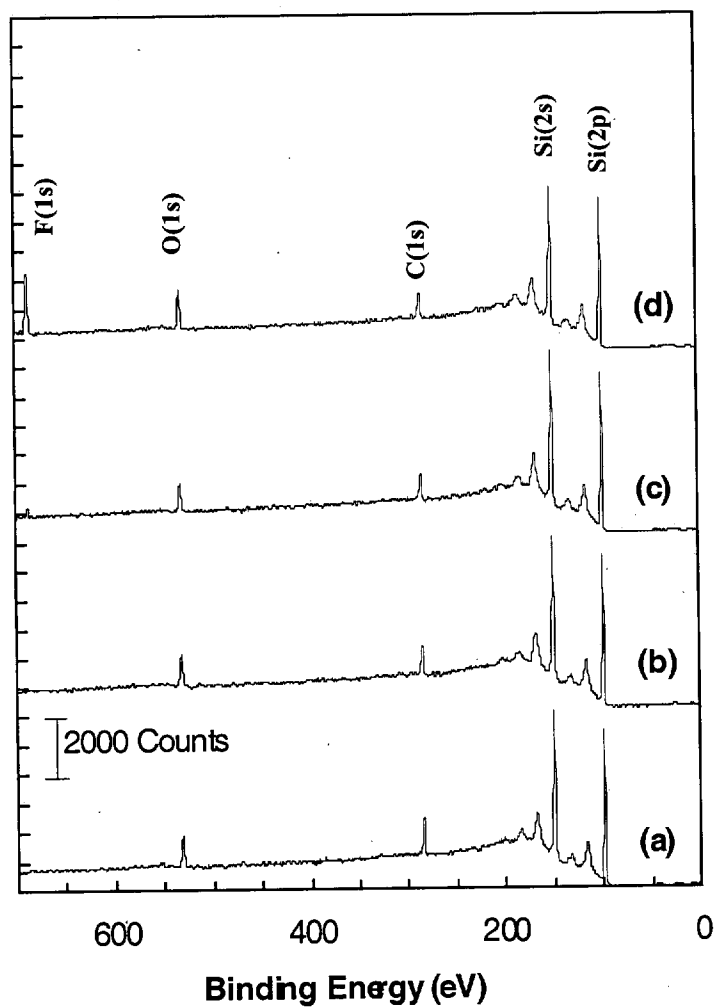


Figure 14. XPS survey spectra of a Si(111) ATR crystal after (a) etching in N_2 -sparged 40% $NH_4F(aq)$, (b) immersion for 5 min in $HO(CH_2)_3CF_3$, (c) immersion for 3-5 min in $HO(CH_2)_3CF_3$ containing 200 mM ferrocene, (d) immersion for 3-5 min in $HO(CH_2)_3CF_3$ containing 200 mM ferrocenium $[BF_4]$.

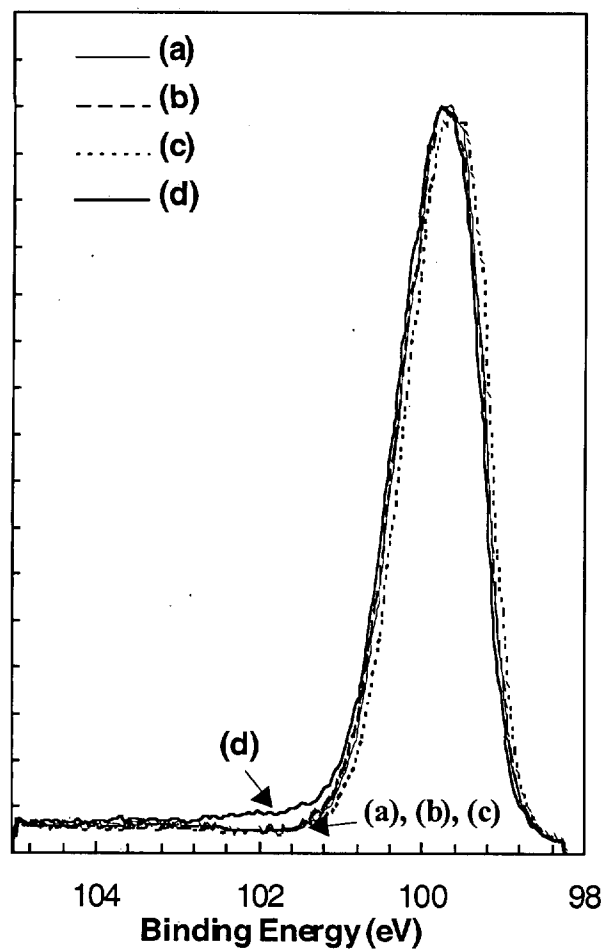


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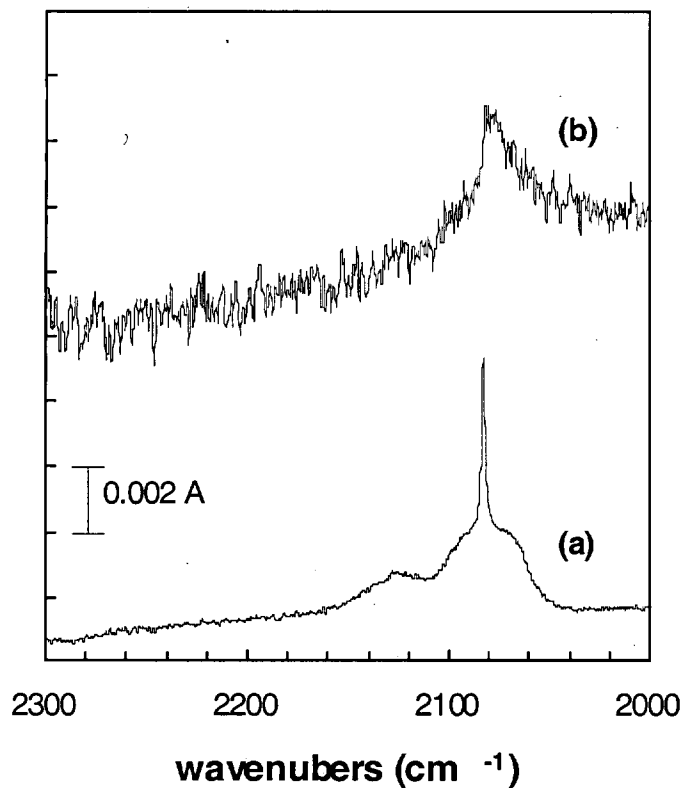


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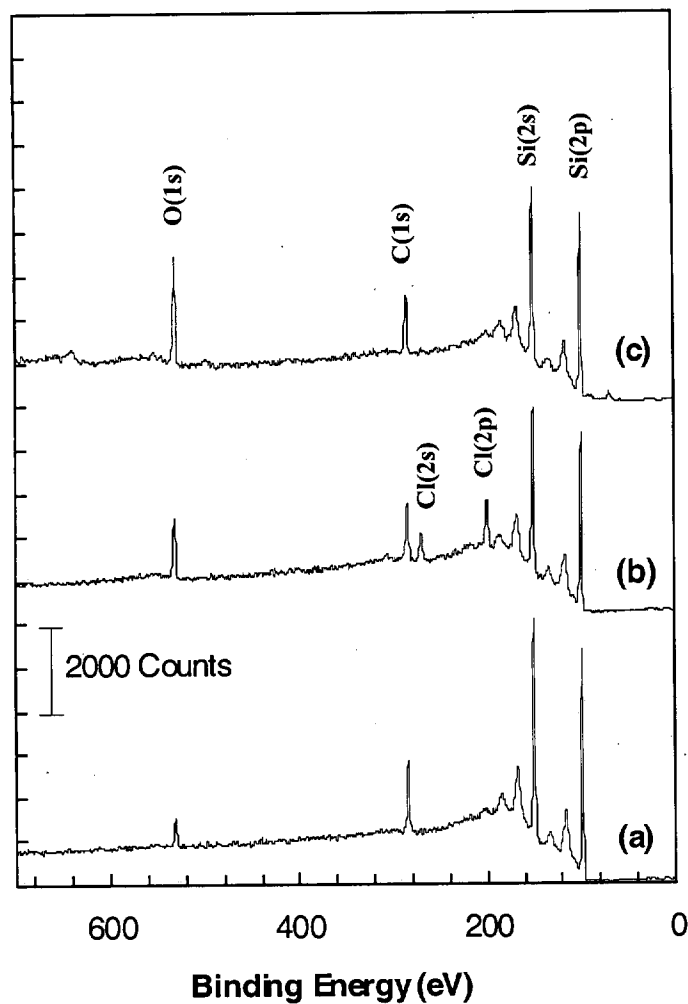


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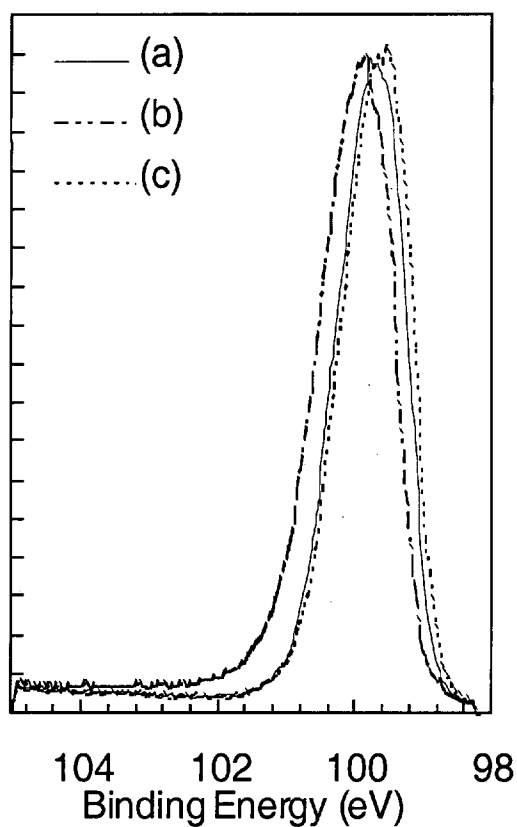


Figure 18. Normalized high-resolution Si 2p spectra of a Si(111) ATR crystal after (a) etching in N_2 -sparged 40% $NH_4F(aq)$, (b) immersion in a saturated C_6H_5Cl solution of PCl_5 at $90^\circ C$ for 50 min, (c) reaction of the chlorinated surface in CH_3OH containing 1.0 M $LiOCH_3$ at $70^\circ C$ for 19 h.

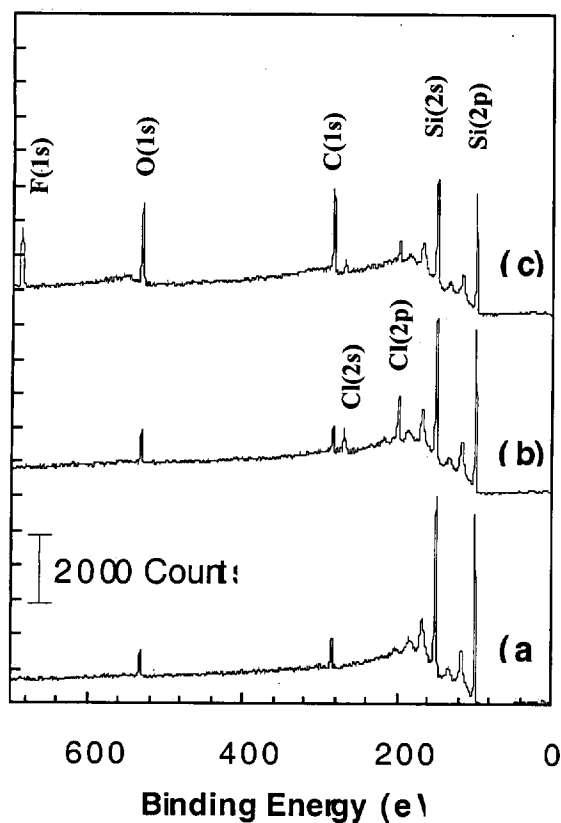


Figure 19. XPS survey spectra of a Si(111) ATR crystal after (a) etching in N_2 -sparged 40% $NH_4F(aq)$, (b) immersion in a saturated C_6H_5Cl solution of PCl_5 at $90^\circ C$ for 50 min, (c) reaction of the chlorinated surface in THF containing 1 M $LiO(CH_2)_3CF_3$ at $80^\circ C$ for 16 h.

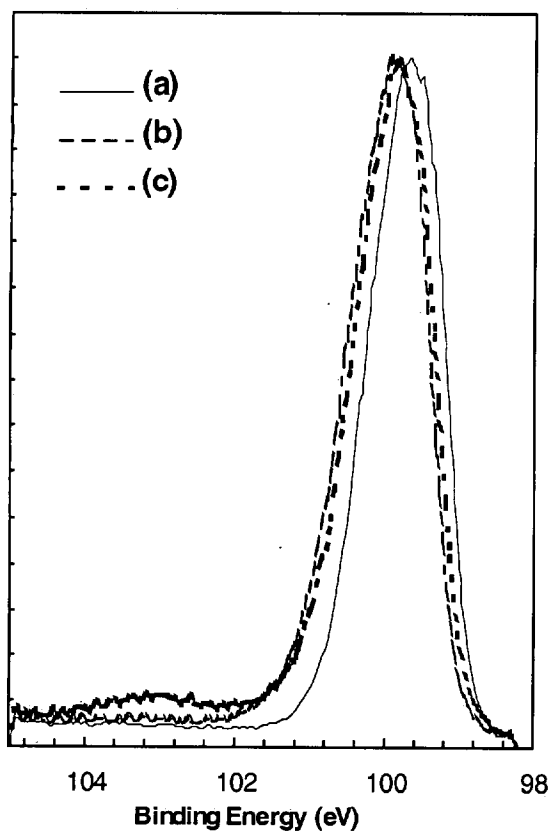


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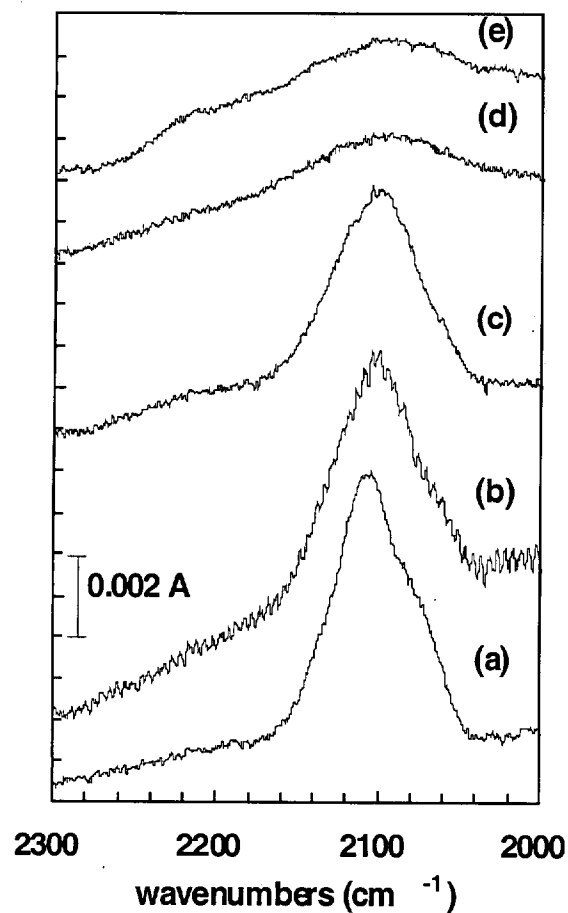


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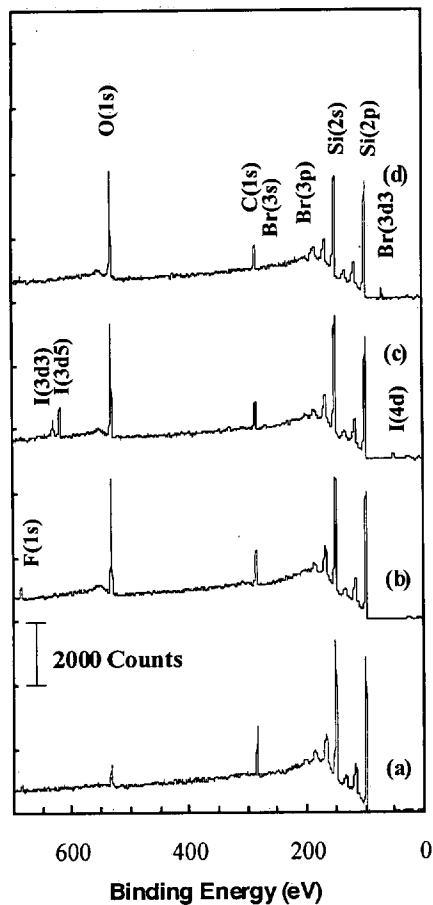


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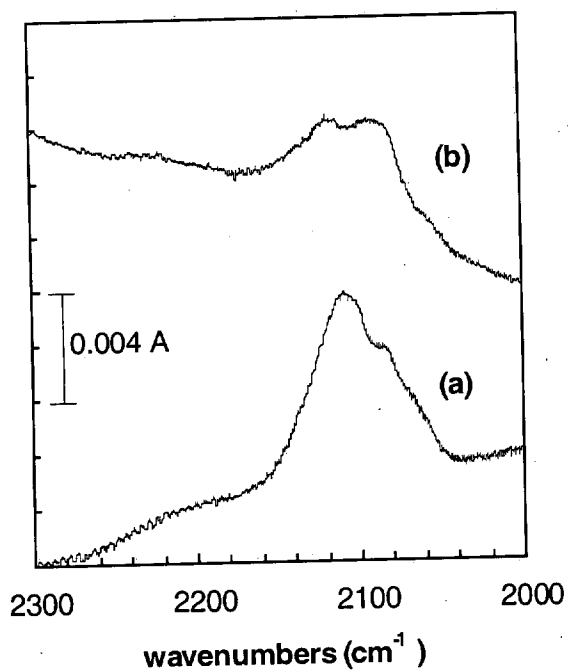


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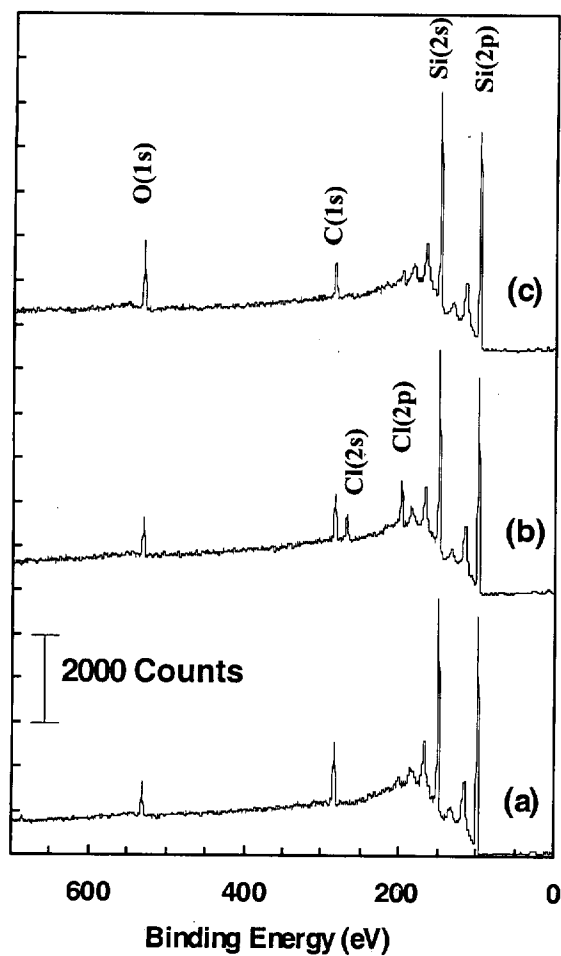


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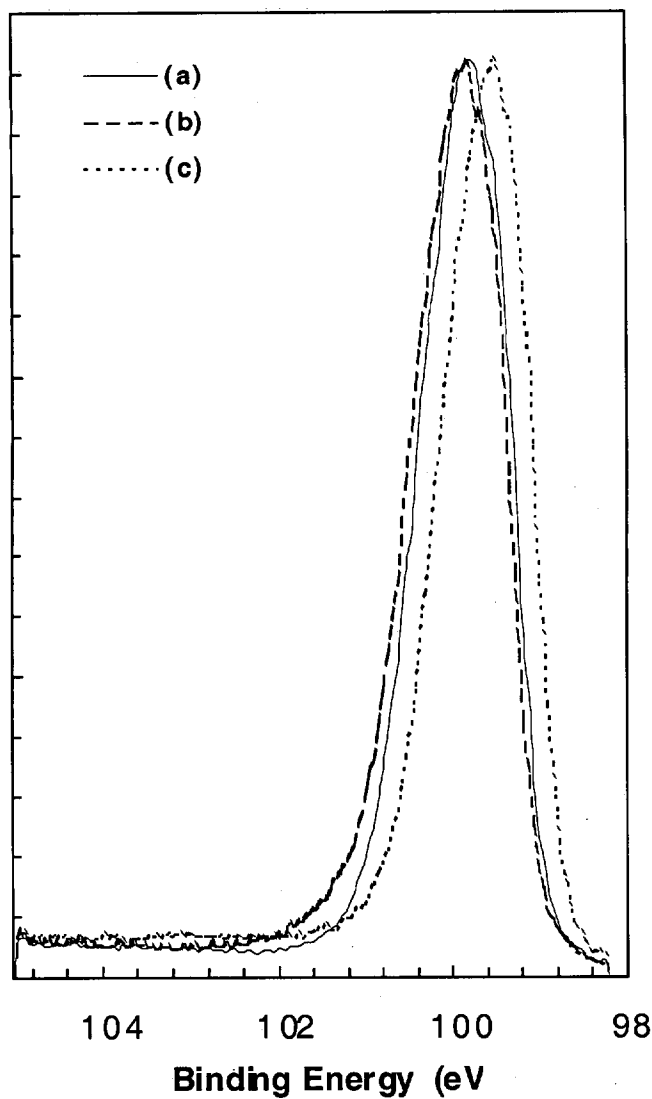


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