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The Theoretical Study of Si Core Levels for the Change of Oxidation State

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The investigations of Si 1s and 2p photoelectron spectra of a poly-Si plate with natural oxide layers based on high energy excitation using X-ray tubes with three kinds of target (Mg K_α, Zr L_α and Ag L_α) and on the theoretical calculations using DV-Xα were presented. From the comparison between the shift values of Si 1s and 2p corresponding with the metal and oxide, it was found that 1s shift is larger than 2p shift. From the discussion on the cluster calculation, the data revealed that the direction of chemical shift is dominated by the change of the population of 3s/3p or 3d independently.

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