# IV-M Photoelectron Spectroscopy of Organic Solids in Vacuum Ultraviolet Region

## IV-M-1 Calculation of Photoelectron Angular Distributions from ω-(n-pyrrolyl)alkanethiol Self-Assembled Monolayers for Different Molecular Orbitals of Pyrrole Group

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We calculated photoelectron angular distributions from ω-(n-pyrrolyl)alkanethiol self-assembled monolayers (pyrrolyl-SAMs) for different π molecular orbitals, $\pi_N$ and $\pi_C$, originating from the pyrrole group. The calculations were carried out within a single-scattering approximation of photoemission process. In the approximation, the photoelectron intensity is caused by not only the self-scattering waves from a pyrrole group but also the single-scattering waves scattered in the vicinity of the pyrrole group. Therefore, the angular patterns involve information on the surface arrangement of the pyrrole groups as well as the character of the molecular orbitals.

## IV-M-2 Calculated Photoelectron Angular Distributions of ω-(n-pyrrolyl)alkanethiol Self-Assembled Monolayers for Distinction between Different Arrangements of Pyrrole Groups

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Photoelectron angular distributions from ω-(n-pyrrolyl)alkanethiol self-assembled monolayers (SAMs) were calculated within a single-scattering approximation of photoemission process. The calculations were carried out on two different surface structures with face-stacked and herringbone arrangements of the pyrrole groups which were deduced from molecular dynamics calculations. The characteristic angular patterns calculated for the molecular orbital originating from the pyrrole group involve information on the orientations of the pyrrole groups, which allows the distinction between these arrangements. The photoelectron angular distributions from the substituted SAMs can be used as a clue for studying the surface structures of the substituent groups.