Organic molecular crystal surface analysis method using photoelectron momentum map

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Picene molecular crystal (C22H14) has a wide band gap and is used as a transistor.It has also been reported that it shows superconductivity by doping a metal element, and its structure and adsorption state on the substrate have been extensively studied.
Puschnig reported that the wave function of adsorbed molecules could be obtained from the Fourier transform of photoelectron angle distribution (PAD) of Angle-resolved photoemission spectroscopy (ARPES) [1]. And many studies have been reported [2-4]. the intensity of PAD, there is a plane wave approximation in which matrix element of the perturbation 'electron photon interaction' between the initial state and final state (plane waves) is calculated.In addition, calculation methods based on multiple scattering has been reported in consideration of intra-molecular scattering of photoelectrons [3,4].
In this presentation, we will report calculation of Picene molecular 's PAD by multiple scattering method in order to take photoelectron scattering from the substrate into consideration.We find the PAD depended on Picene molecular 's adsorption position and adsorption distance. We will discuss PTCDA, which is well known about the collective arrangement on the substrate, too.

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