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The XPS core spectral functions of free and physisorbed molecular oxygen

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Abstract

A model for calculating X-ray photoelectron spectral functions in physisorbed systems is proposed and applied to molecular oxygen (O₂) on graphite. The polarization interaction is found to be selective with respect to the final state and with respect to the orientation of the adsorbate leading to small but distinct changes in the vibronic coupling constants and spectral functions. The characteristics of the X-ray photoelectron spectrum of free oxygen are investigated at several levels of approximation.

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