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Time-dependent surface electronic structure of EuB₆

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for the next step - multiple fragmentation processes of large molecules.

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O11

Vibrationally Resolved Molecular-Frame Photoelectron Angular Distributions in the Core-Level σ Shape Resonance Regions for CO₂ and CO Molecules

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We have measured molecular-frame photoelectron angular distributions (MFPAD) for the vibrationally resolved (VR) 1s photoelectrons from CO₂ and CO [1] molecules in the σ shape resonance regions. The VR-MFPAD's for the $v_3 = 0$, and 1 levels in the $O1s \rightarrow \epsilon l\sigma$ channel for CO₂ molecules are different each other at the incident photon energies; 545 eV (near the σ_g^* resonance), 553 eV, and 561 eV (on the σ_u^* resonance). In the case of the CO₂ molecule, the activated vibrational mode is the anti-symmetric stretching mode due to the dynamic core-hole localization (or the vibronic coupling) [2]. Then, we can not directly relate the mode with the dissociative coordinate. This is different from the case of CO molecules in the way of the vibrational effect in the photonionisations. We will discuss the mechanism of the vibrational effect on the VR-MFPAD's for the CO₂ molecule in comparison with the case of the CO molecule [1].

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O12

Time-dependent Surface Electronic Structure of EuB₆

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The surface electronic structure of UHV-cleaved divalent hexaboride EuB₆ is investigated using angle-resolved photoemission. A time-dependent filling of a small X-point electron pocket of Eu 4d-character is correlated to changes in the overall B-p band structure and Eu 4f states. The X-point electron pocket size is observed to initially increase in size and then recede to zero occupation. Similarly a Eu 4f component is observed to initially increases in binding energy and then reverses direction and loses intensity. Surface-slab LDA calculations allow identification in the data of (i) a distinct surface-related band residing in the bulk-projected band gap along X-M and (ii) energyshifted surface-atom Eu 4f states resulting from an electric dipole at the highly ionic surface. The experimental time-dependent behavior is explained in terms of clustering of mobile surface Eu atoms on the freshly cleaved surface, followed by adsorption of residual gases. The understanding of these surface effects has also allowed deeper insight into the bulk electronic structure and ferromagnetic ordering below ~ 15 K, which are discussed in relation to other nonmagnetic divalent hexaborides that have been determined by ARPES to be ~ 1 eV band gap semiconductors [1].

Acknowledgments

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