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Quantum-mechanical simulation of attosecond streaked photoemission from Mg-covered W(110) surfaces

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Synopsis We apply a quantum-mechanical model to simulate infrared-streaked photoelectron emission by an ultrashort extreme ultraviolet pulse from adsorbate-covered metal surfaces. Incorporating effects of energy-dependent electron mean-free paths, the properties of initial states, photoelectron energy dispersion, and the screening of the streaking field, this model is able to reproduce recently measured photoelectron spectrograms and adsorbate-thickness-dependent photoemission time delays.

Attosecond streaking, using an isolated attosecond extreme ultraviolet (XUV) pump pulse and a delayed few-cycle infrared (IR) streaking pulse, is able to time-resolve electron photoemission from atoms and condensed matter systems on an attosecond time scale [1]. A recent streaked photoemission experiment with ultrathin Mg adsorbate films on a W(110) substrate [2] reveals a monotonic dependence of the relative photoemission time delay $\Delta\tau_{4f-2p}$ between W($4f$) and Mg($2p$) core-level (CL) photoelectrons and a non-monotonic dependence of the relative photoemission time delay $\Delta\tau_{CB-2p}$ between conduction band (CB) and Mg($2p$) CL photoelectrons on the adsorbate thickness.

In order to interpret the measured relative photoemission time delays from the Mg/W(110) systems, we apply a quantum-mechanical model [3, 4]. By taking the energy-dependent electron mean-free path (MFP), the properties of initial states (including band-structure and wave-function-localization effects), energy dispersion, and the screening of IR streaking field at the surface into account, our numerical results [5] reproduce measured [2] streaked photoemission spectra and relative photoemission time delays as a function of the Mg-film thickness (Fig. 1).

As input for our numerical simulation, we only employ measured and calculated MFPs and an IR skin depth of 2 Å [2, 3]. In addition, we describe the dispersion of released CB electrons inside the W substrate based on an adjusted effective electron mass (0.86 a.u.). We assume free-electron propagation of CB electrons in the Mg adsorbate film and for electrons that are released from Mg($2p$) and W($4f$) CLs, to match the relative photoemission delay between CB and W($4f$) photoelectrons for the adsorbate-free W(110) surface. Our quantum-mechanical results also agree with classical free-electron calculations [2] for $\Delta\tau_{4f-2p}$.

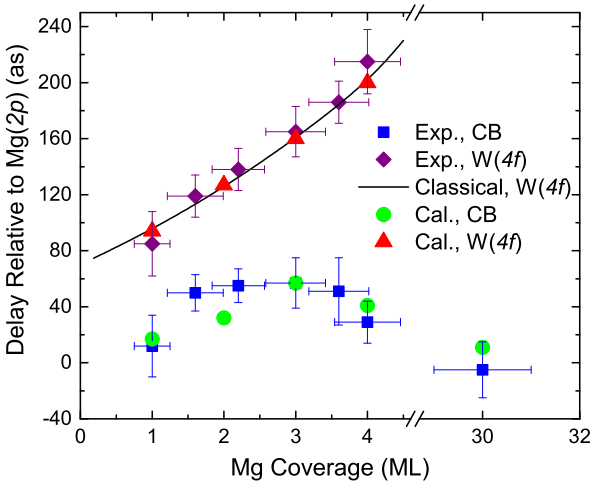

Figure 1. Measured [2] and classically [2] and quantum-mechanically [5] calculated streaking time delays relative to Mg($2p$) emission for CB and W($4f$) photoelectrons as a function of the Mg coverage on a W(110) substrate. The central XUV photon energy is 118 eV.

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