

SUPPORTING INFORMATION

Electronic Signatures of a Model Pollutant-Particle System: Chemisorbed Phenol on TiO₂(110)

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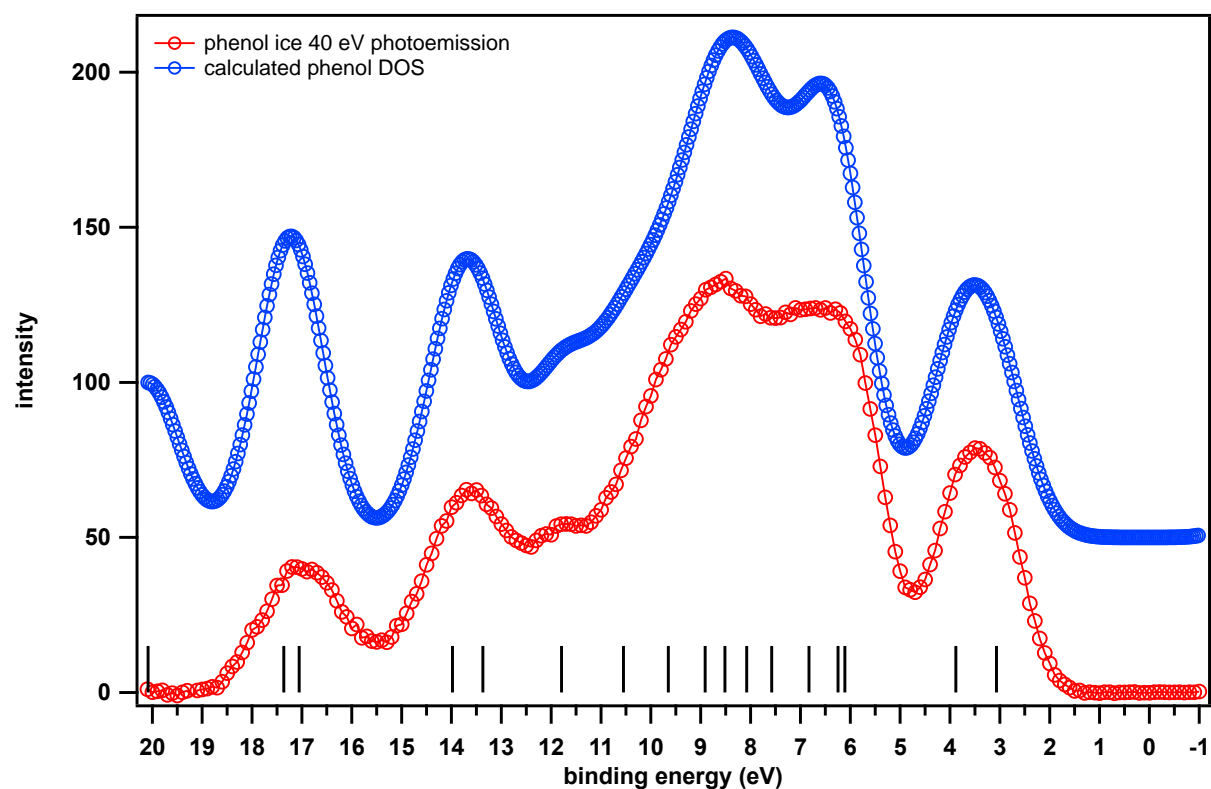


Fig. S1 Comparison of photoemission spectrum from phenol ice (red) under the same conditions as in Fig. 1 (40 eV photon, -173°C) with a calculated DOS for a single phenol molecule (blue). The positions of the calculated molecular orbitals are indicated by the black vertical bars.

We have subtracted the secondary electron background from the experimental data to facilitate comparison with a calculation. The calculated eigenvalues and density of states have been rigidly shifted by 2.9 eV towards lower binding energy to align the phenol HOMO orbital with the lowest energy photoemission peak. The agreement between the calculated DOS and the photoemission spectrum is excellent.

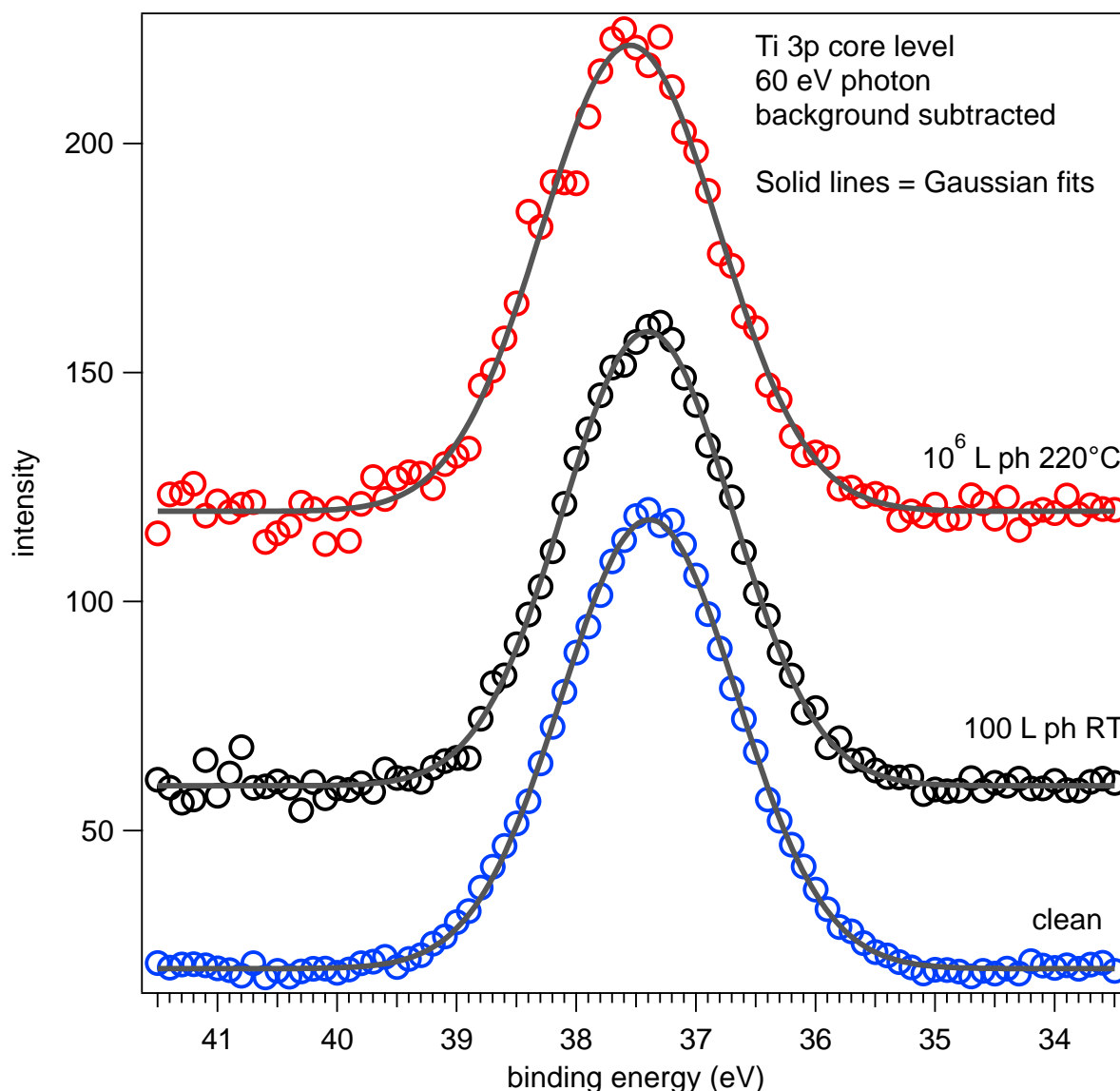


Fig. S2. Ti 3p core levels acquired under phenol dosing conditions discussed in this work – clean TiO_2 (blue, bottom), 100 L phenol dosed at room temperature (black, middle), and 10^6 L phenol dosed at 220°C (red, top). All spectra were acquired at a photon energy of 60 eV. Open circles show the experimental data after the removal of the secondary electron background, and solid lines show a single Gaussian function fit to each respective peak; the FWHM of the fitted peaks was a free parameter, but did not vary with dosing condition. The binding energies from the Gaussian fits are as follows (uncertainties expressed as one standard deviation):

Clean oTiO_2 :	37.39 ± 0.004 eV
100L phenol RT:	37.41 ± 0.006 eV
10^6 L phenol 220C:	37.55 ± 0.011 eV

The shift to higher binding energy of the Ti 3p peak after a high temperature phenol dose is taken as a sign of band bending and has been used in the analysis of difference spectra in Figs. 1-2.

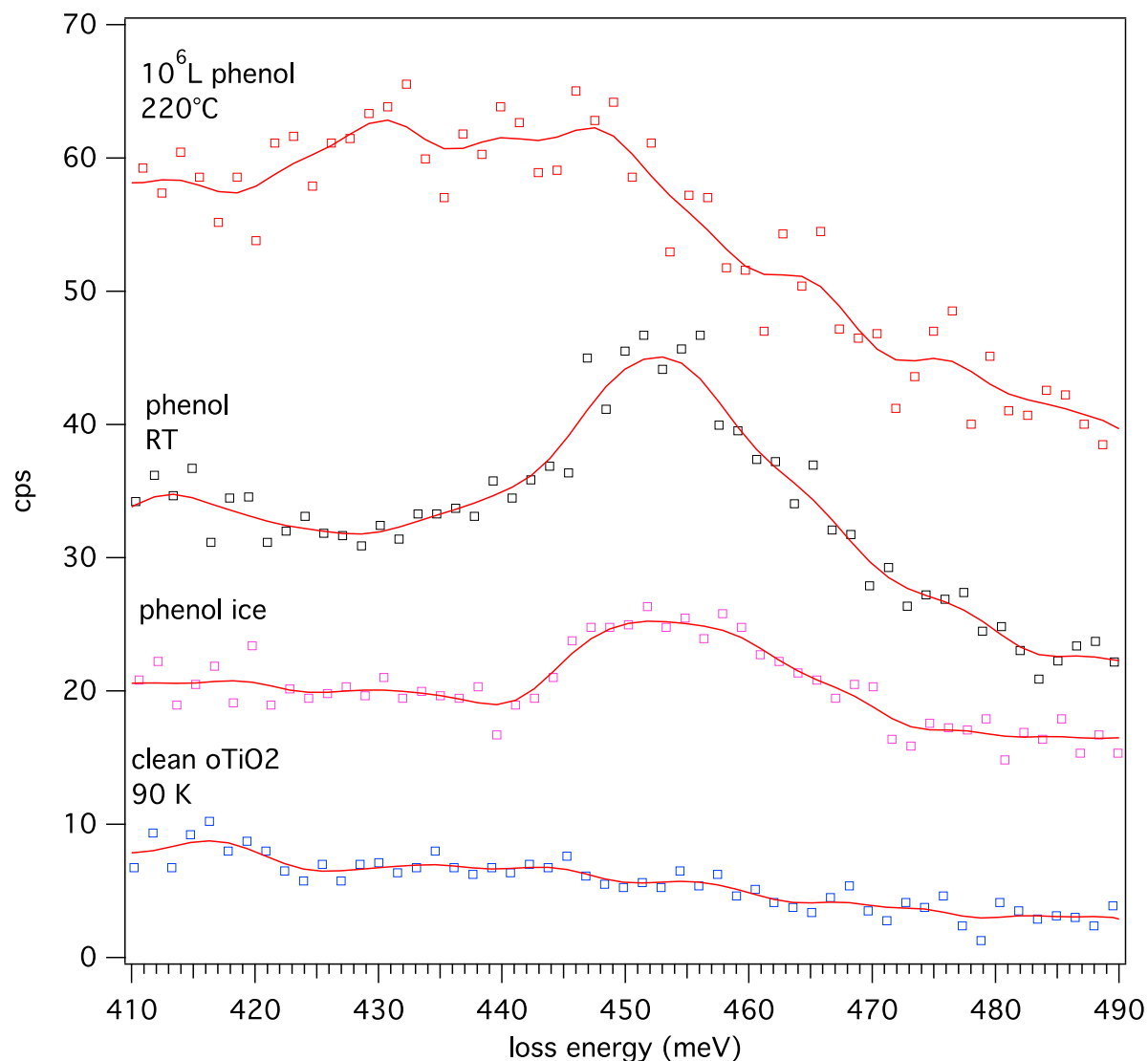


Fig. S3 Vibrational EELS spectra of the O–H stretching region of phenol/TiO₂ under the dosing conditions discussed in this work. For the vibrational EELS measurements, the primary beam energy was 7 eV and the overall energy resolution was 10 meV. The clean o-TiO₂ and phenol ice spectra were acquired with the sample held at 90K; the room temperature and high temperature phenol doses were acquired with the sample at room temperature after dosing. Open symbols represent the data; solid lines show the data smoothed by a binomial algorithm. Spectra are normalized to the elastic peak (not shown) and vertically offset for clarity.