Supporting Information:

D_2O Interaction with Planar ZnO(0001) Bilayer Supported on Au(111): Structures, Energetics and Influence of Hydroxyls

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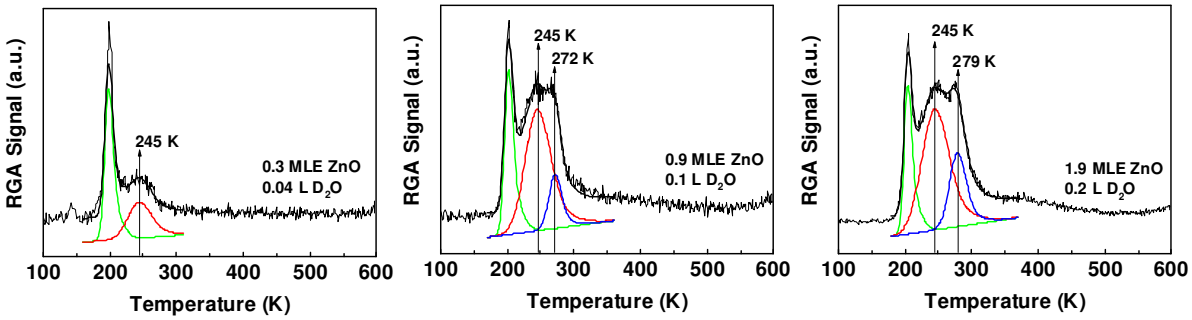

Figure S1. Examples of fittings of the TPD traces to semi-quantify the relative amount of D_2O that saturates desorption peaks β and γ. For simplicity, the fitting has been performed using components of mixed Gaussian-Lorentzian functions. Only the peak positions were constrained for the fitting. The intensities and the full width at half maxima of the components were optimized.

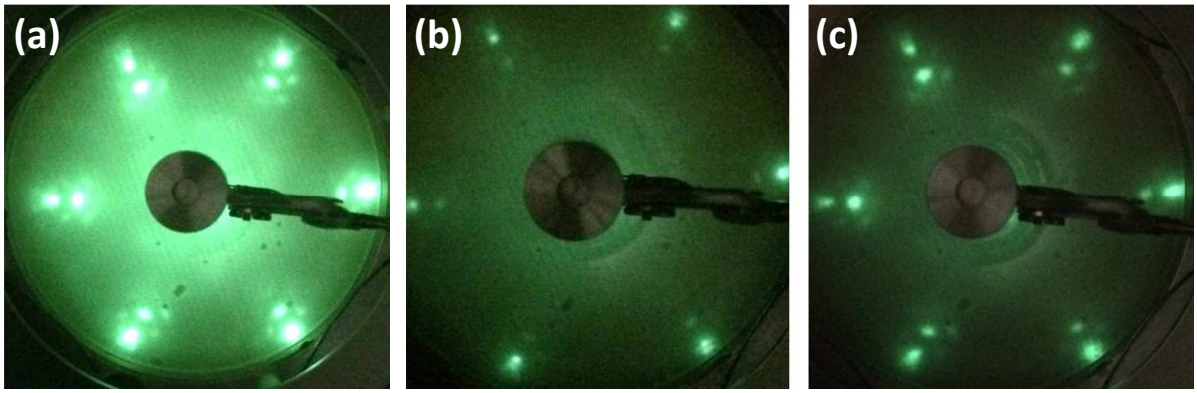

Figure S2. LEED patterns of (a) the clean 1.1 MLE ZnO(0001) bilayer on Au(111) showing a coincidence structure of ZnO(0001)-(7 × 7)/Au(111)-(8 × 8); (b) after an exposure of 0.3 L D_2O on 1.1 MLE ZnO at T = 100 K; and (c) after heating to T = 600 K. All LEED patterns were obtained at T = 100 K with a beam energy of 42 eV.