

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

***GW* at the interface: CH₃OH and H₂O on TiO₂(110)** DUNCAN MOWBRAY, ANNAPAOLA MIGANI, AMILCARE IACOMINO, Universidad del Pais Vasco UPV/EHU, E-20018 San Sebastian, Spain, JIN ZHAO, University of Science and Technology of China, Hefei, Anhui 230026, China, HRVOJE PETEK, University of Pittsburgh, Pittsburgh, Pennsylvania 15260, USA, ANGEL RUBIO, Universidad del Pais Vasco UPV/EHU, E-20018 San Sebastian, Spain — Electronic level alignment at the interface between an adsorbed molecular layer and a semi-conducting substrate determines the activity and efficiency of many photocatalytic and photovoltaic materials. However, a quantitative description of the states at the interface remains elusive, due to the computational complexity of quasiparticle *GW* based algorithms. We compare density functional theory (DFT) calculations and quasiparticle techniques with ultraviolet photoelectron spectra and two photon photoemission spectra to determine the level of theory required to obtain an accurate description of occupied and unoccupied states at the interface. Specifically, we consider GGA DFT, hybrid DFT and G_0W_0 , *scGW*1, *scGW*₀, and *scGW* quasiparticle calculations for the interface between rutile TiO₂(110) and methanol or water. We find the quasiparticle energy shifts Δ are linearly dependent on the fraction of the wave function density within the molecular layer f_{mol} and the bulk substrate f_{bulk} . For the unoccupied states, the same correlation holds for all the molecular layers studied. This allows one to describe the quasiparticle energy shifts semi-quantitatively for larger molecular layers on TiO₂(110) based on more tractable DFT calculations.

Duncan Mowbray
Universidad del Pais Vasco UPV/EHU, E-20018 San Sebastian, Spain

Date submitted: 13 Nov 2012

Electronic form version 1.4