Raman study of SP6* adsorbed on oxide surfaces

*2,7-bis(biphenyl-4-yl)-20,70-di-tert-butyl-9,9'-spirobifluorene

In order to exploit the potential of organic/inorganic semiconductor hybrid structures, control over the structural and electronic properties of the hetero-interface is crucial. Interface formation in such hybrid structures is a very complex issue, not least due to dangling bonds, steps, and defects on the inorganic surface. Binding of molecules at such sites can cause modifications of their electronic structure or even their fragmentation resulting in ill-defined interfaces.

In a recent publication of the SFB 951 projects B9 (Stähler/Wolf) and B4 (Knorr/Rinke/Scheffler) the vibrational properties of SP6 on ZnO(000-1), ZnMgO(000-1), and Al_2O_3(11-20) substrates were investigated by non-resonant Raman spectroscopy.

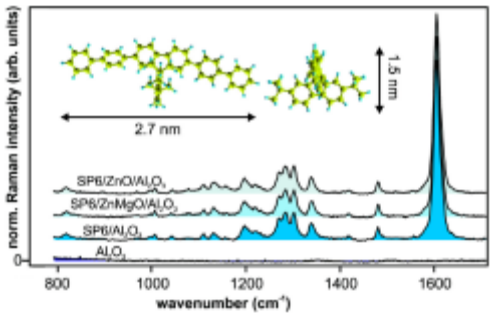

Fig. 1: Raman spectra of 8 nm SP6 on sapphire, ZnMgO(000-1), and ZnO(000-1). The bottom spectrum depicts the sapphire response for comparison. Inset: SP6 molecule as calculated by DFT.

Figure 1 shows the Raman spectra of 8 nm SP6 deposited onto the different substrates as well as the Raman response of the bare sapphire substrate itself. All SP6 spectra in Figure 1 are dominated by a band around 1300 cm^{-1} and a peak at 1600 cm^{-1}. DFT calculations of isolated gas phase molecules allowed the assignment to CC-stretch and ring stretch modes, respectively. Remarkably, the substrate does not influence the vibronic response of the few monolayer thick SP6 film.

The substrate's impact on the vibrational properties of the first SP6 monolayer is focused on in Figure 2. It shows the Raman spectra of 1.0 nm SP6 layer on ZnO (a), and on Al_2O_3(11–20) (b, blue). Subtraction of these spectra leads to a trace coinciding with the Raman response of ZnO(000-1) (c). If this this substrate-induced background is subtracted from the spectrum of 8.0 nm SP6/ZnO(000-1) and divided by 8, the resulting trace (b, orange) coincides almost perfectly with the spectrum of 1.0 nm SP6/ Al_2O_3(11–20). This shows that there is no influence of the substrate on the Raman response of SP6 confirming that the electronic structure of SP6 is not perturbed by interaction with the substrate surface.

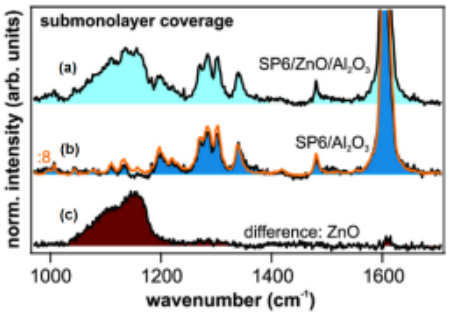

Fig. 2: Comparison of 1.0 nm SP6 (mass equivalent) on ZnO(000-1) and sapphire showing that there is no substrate-induced difference in the response of the molecules. The band between 1050 and 1200 cm-1 results from phonons in the ZnO(000-1) film. The signal of 8.0 nm SP6 on ZnO(000-1) matches the 1.0 nm SP6/Al_2O_3 (11-20) trace after subtraction of the ZnO(000-1) signal and scaling by a factor of 8 (orange curve).

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