Making natural materials clean – and model samples dirty.

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To improve interpretion of experimental geochemical data, simulations are used. However, theoretical approaches require a certain number of assumptions; otherwise computational requirements become astronomical. Thus, molecular models usually use flat or minimally stepped, pure, "clean" surfaces, e.g., no carbon contamination of the sort that comes from the environment, called "adventitious carbon" (AC). AC is extremely difficult to remove and ubiquitous on all mineral surfaces exposed to air or water.

However, surface analysis with X-ray photoelectron spectroscopy (XPS) and atomic force microscopy (AFM) clearly demonstrate that such a layer modifies the reactivity of quartz (SiO_2) surfaces. New density functional theory (DFT) modelling of carbon containing compounds on calcite surfaces also supports previous XPS results - that AC can change the affinity of the surface for organic molecule attachment, even simple alcohols..

We have developed a fast and easy method for producing "clean" surfaces analogous to those used in modelling (Figure 1) which does not change surface structure. Combined with the development of organic self assembled (SAM) monolayers, for use in deriving experimental data of a model "dirty" system that can be explored theoretically, we can begin to bridge the gap between experiments and models.

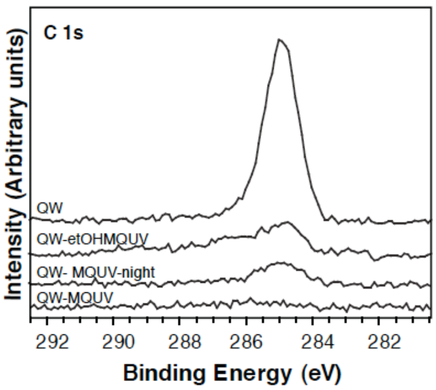

Figure 1: XPS C 1s spectra from quartz wafers (QW) treated (with ethanol (etOH), MilliQ water (MQ) and UV ozone (UV)) to remove the adventitious carbon peak at 285.0 eV.

The Carnian Pluvial Event negative CIE at Cave del Predil (early Late Triassic, Italy): a new link to Wrangellia volcanism

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A ~4‰ negative C-isotope excursion (CIE) in higher plant *n*-alkanes has recently been discovered coincident with the onset of the Carnian Pluvial Event (CPE) [1], during which a major climatic and biotic turnover occurred [2]. This C-cycle disturbance has been linked to the eruption of the Wrangellia oceanic plateau (western North America), a Large Igneous Province (LIP) that is thought to have extruded up to 1 million cubic kilometres of basalts during the early Late Triassic [3].

C-isotope analyses of bulk organic matter from stratigraphic sections in the Cave del Predil area (Julian Alps, north eastern Italy) reveals an early Carnian ~6‰ negative CIE corresponding to the onset of the CPE [4]. The negative CIE occurs just below the level recording the first major terrigenous input and change in vegetation type to a hygrophytic flora that can be correlated with the existing stable C-isotope curve from the Dolomites [1].

Our new data show that the major negative CIE at the onset of the CPE can be correlated at least regionally and likely represents a global signal. This C-cycle perturbation could have been caused, directly or indirectly, by the release of large amounts of CO_2 during the coeval eruption of the Wrangellia LIP that led to the Carnian climatic, environmental and biological changes.

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