Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Interaction of the ionic liquid [BMP][TFSA] with rutile TiO_2(110) and coadsorbed lithium

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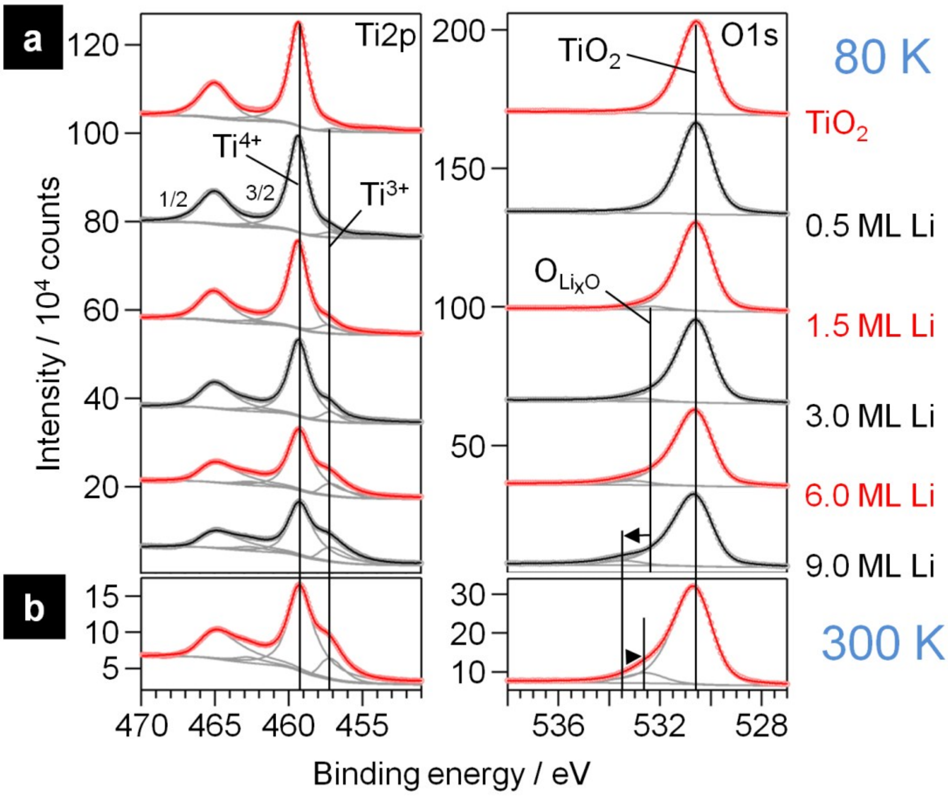

Figure S1: (a) XP detail spectra from the same experiment as the ones shown in Fig. 4, but taken at 0° detection angle: (a) clean TiO_2 (topmost spectra) and increasing amounts of Li evaporated onto this surface. (b) XP spectra recorded after slowly heating the sample overnight to 300 K.

The thickness of the Li_xO overlayer was calculated following ref. [1]:

$$I_{Li_xO} = I_{Li_xO,\infty} \cdot \left[1 - exp\left(-\frac{d}{\lambda_{O1s\,Li_xO,Li_xO} cos\theta}\right)\right] \tag{1a}$$

$$d = -\lambda_{O1s\,Li_xO,Li_xO} \cdot cos\Theta \cdot ln\left(1 - \frac{I_{Li_xO}}{I_{Li_xO,\infty}}\right) \tag{1b}$$

where d is the thickness of the overlayer, λ the mean free path of the emitted electrons from the O1s peak in Li_xO damped by Li_xO and θ the detection angle relative to the surface normal, $I_{Li_xO,\infty}$ the intensity of the O1s signal of bulk Li_2O and I_{Li_xO} the O1s intensity originated by the Li_xO layer. λ is calculated to be 2.52 nm from the NIST electron effective attenuation length database[2] which is based on calculations by Powell et al. and measurements by Jablonski et al.[3,4]. This gives a mean escape depth of 0.5 nm when measuring at 80°. The mean escape depth is defined following ref. [5]. Θ is corrected for the refraction of the emitted photoelectron wave at the surface barrier from 80° to 77.2° following refs. [6,7]. $I_{Li_xO,\infty}$ is calculated from the bulk O1s rutile signal by taking into account the difference in stoichiometry of oxygen per formula unit, in the density of the materials and in the EALs following ref. [1].

Alternatively the thickness was calculated using the damping of the O1s(LTO) or the Ti2p signals, following ref. [1]:

$$I_{LTO} = I_{LTO,\infty} \cdot exp\left(-\frac{d}{\lambda_{Ti2p/O1s\,LTO,Li_xO} cos\theta}\right) \tag{2a}$$

$$d = \lambda_{Ti2p/O1s\,LTO,Li_xO} \cdot cos\Theta \cdot ln\frac{I_{LTO,\infty}}{I_{LTO}} \tag{2b}$$

where I_{LTO} is the intensity of the Ti^{4+}+Ti^{3+}/O1s(LTO) peaks, $I_{LTO,\infty}$ the ones calculated for bulk LTO (analogously to $I_{Li_xO,\infty}$) and $\lambda_{Ti2p/O1s\,LTO,Li_xO}$ the mean free path of electrons emitted from Ti2p/O1s core levels in LTO in the Li_xO cover layer.

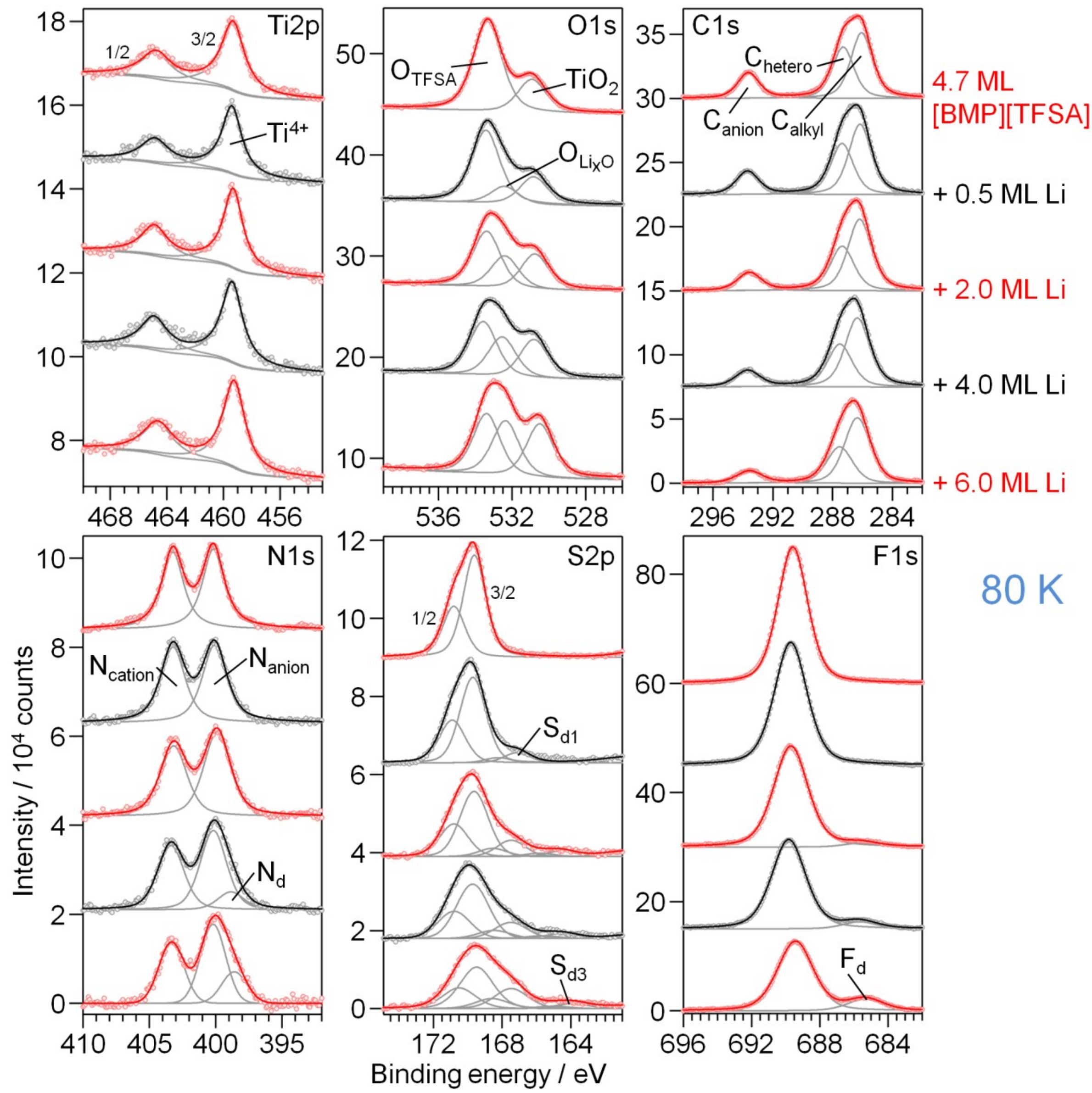

Figure S2: XP detail spectra of 4.7 ML [BMP][TFSA] deposited on $TiO_2(110)$ at 80 K (topmost spectra) and step by step post deposition of 6 ML of Li.

Literature

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