Supporting Information

for

Imaging the surface potential at the steps on the rutile TiO$_2$(110) surface by Kelvin probe force microscopy

Masato Miyazaki, Huan Fei Wen, Quanzhen Zhang, Yuuki Adachi, Jan Brndiar, Ivan Štich, Yan Jun Li and Yasuhiro Sugawara


Details of the DFT calculations
DFT calculations were performed using VASP [1], with the standard PAW pseudopotential (4/6 electrons for Ti/O species), 400 eV plane wave cut-off, and the GGA+U [2] exchange–correlation approximation (U set to 2.5 eV). We use $1 \times 6 \times 1/1 \times 4 \times 1$ k-point sampling of the Brillouin zone for the $\langle 001 \rangle / \langle 1\bar{1}1 \rangle$ step configurations. To construct the different step configurations, we follow the calculations in [3,4]. We use a much larger $\langle 1\bar{1}0 \rangle$ in-plane supercell size to converge the charge redistribution to be able to compare the $\langle 1\bar{1}0 \rangle$ area for different step configurations. Top and side views of the supercells used are shown in Figure 1. We use a six-layer configuration with opposite step configurations to neglect interactions. We use roughly 50 Å separation in the $z$-direction.
Figure 1: DFT simulation supercells for the different step configurations. From top to bottom and left to right (1\(\bar{1}\)1)\(_R\), reduced (1\(\bar{1}\)1)\(_R\), (001)\(_O\), (001)\(_Ti\)
References


