Beyond Ideal Tips and Ideal Surfaces

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Test System

A – 1.8 nm
f_0 – 160 kHz
k – 26 N/m
R – 20 nm

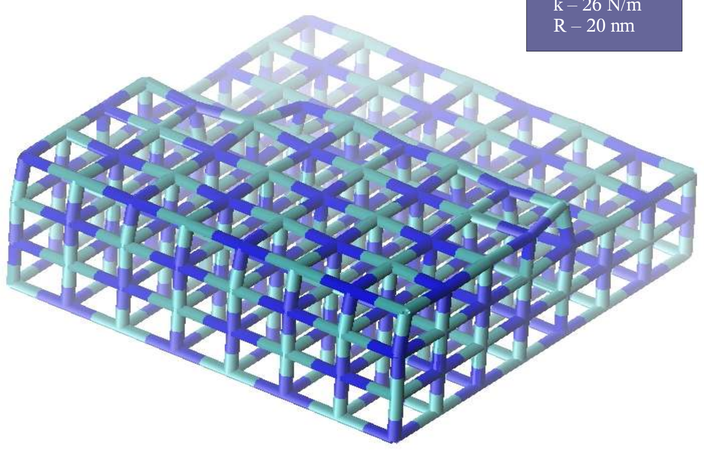

Fig. 1: The NaCl terrace used in simulation. The bottom atom layer is frozen in place. Turquoise denotes Cl and blue Na atoms, so the terrace has both an Na and a Cl kink site.

Ideal tips – single probe

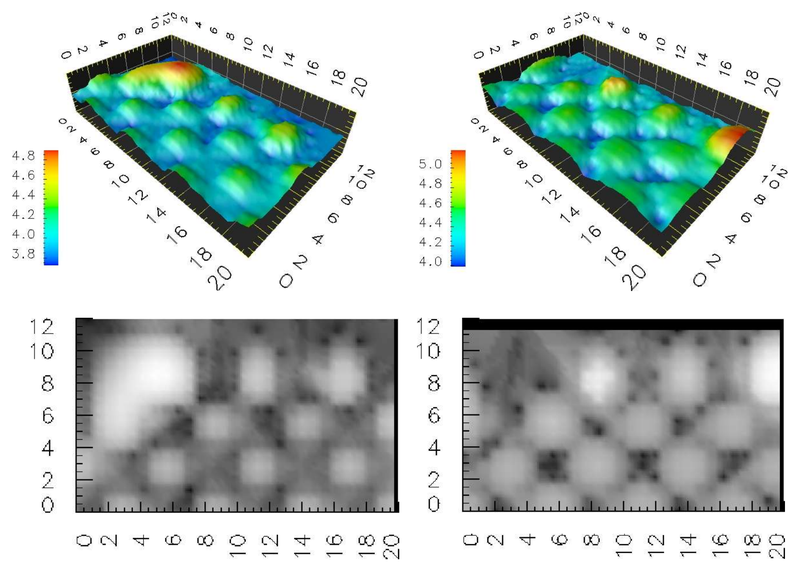

Fig. 2: Simulated images of the island with an ideal NaCl cuboid tip, Cl-terminated (left) and Na-terminated (right).

- Tips with either a Cl or Na at the apex provide clear contrast localized on atomic sites, and increased contrast at step-edges and kinks.

Tips with three atoms down

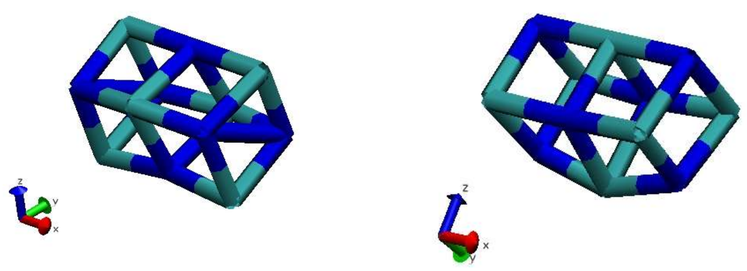

Fig. 3: Simulated tips with three atoms towards the surface: Cl-Na-Cl (left) and Na-Cl-Na (right). The tip is very soft and easily twists sideways, since only the top three atoms are fixed in place.

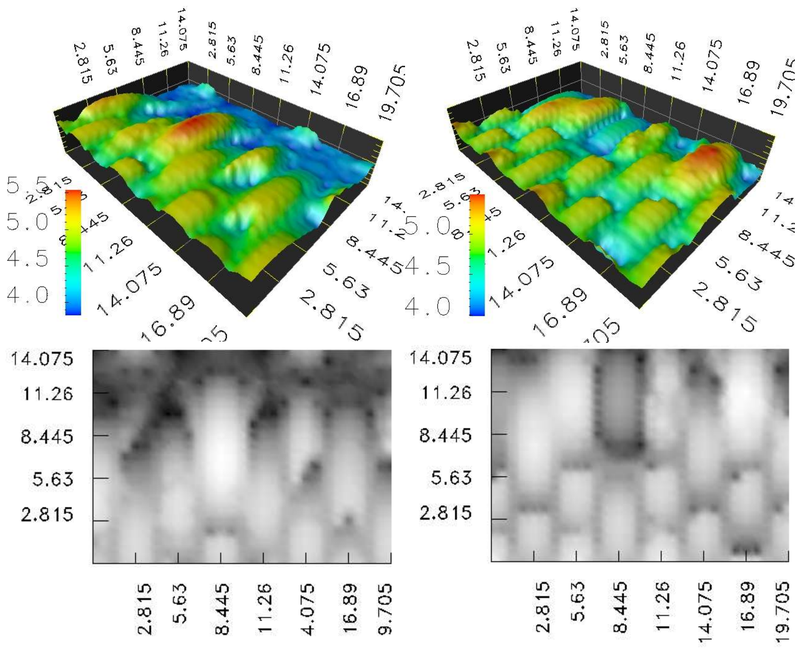

Fig. 4: Simulated results for soft Cl-Na-Cl (left) and Na-Cl-Na (right) terminated tips. Both images are calculated at a frequency change of 140 Hz. Tick marks on pictures mark the rows of atoms; units are Å.

- Softness of the tip allows twisting during scanning, which smears out the contrast.
- Contrast is much smaller than for a standard tip.

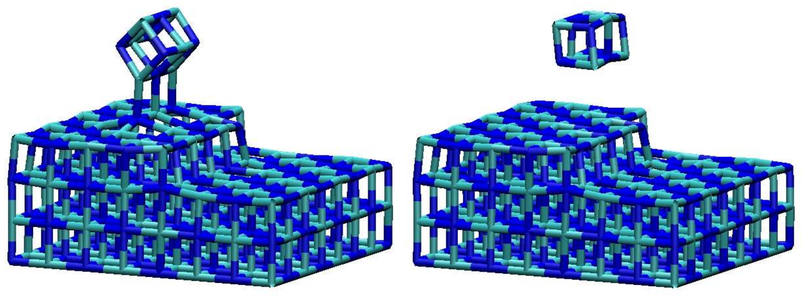

Fig. 5: Layouts of the Cl-Na-Cl tip at the same height but slightly different locations. On the right the tip is twisted about 45 degrees compared to the tip on the left, bringing it higher though the three fixed atoms are at the same height as before.

- Twisting can be reduced by increasing the size of the tip.

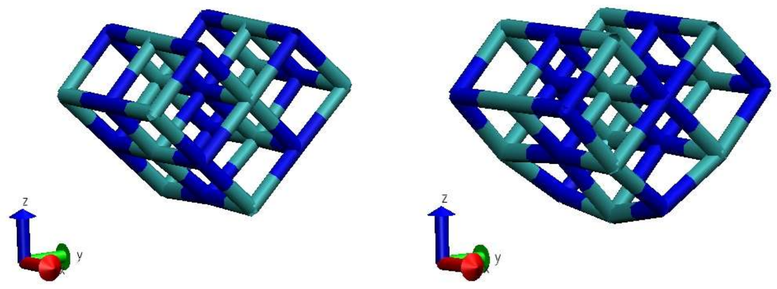

Fig. 7: Simulated tips with three atoms towards the surface: Cl-Na-Cl (left) and Na-Cl-Na (right). The tip is soft, but pivoting is prevented by twelve additional atoms holding the bottom of the tip in place.

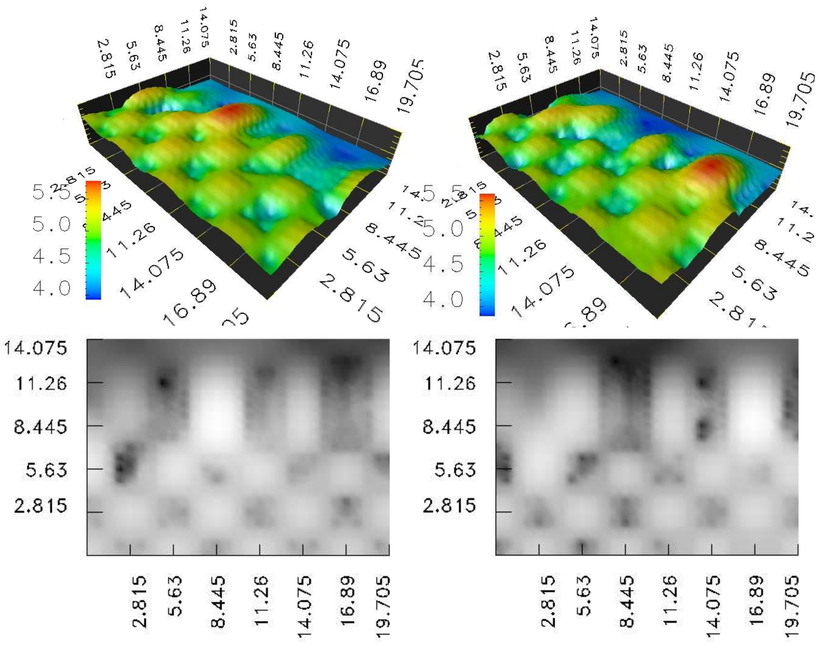

Fig. 8: Simulated results for soft Cl-Na-Cl (left) and Na-Cl-Na (right) terminated tips, with additional atoms to prevent pivoting. Both images are calculated at a frequency change of 120 Hz. Tick marks on pictures mark the rows of atoms; units are Å.

Tips with two atoms down

- Also simulated were 12-atom NaCl tips with an Na-Cl edge down, parallel and perpendicular to the terrace, with 6 top atoms fixed.

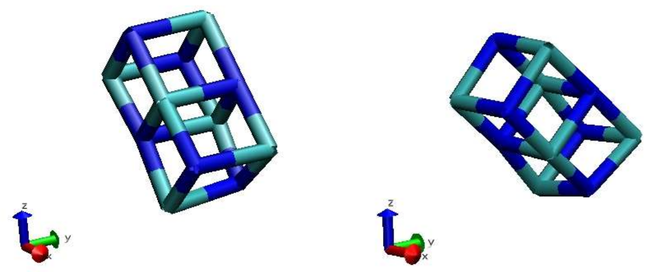

Fig. 9: Simulated tips with two atoms towards the surface: two atom-edge perpendicular (left) and parallel (right) to the simulated terrace.

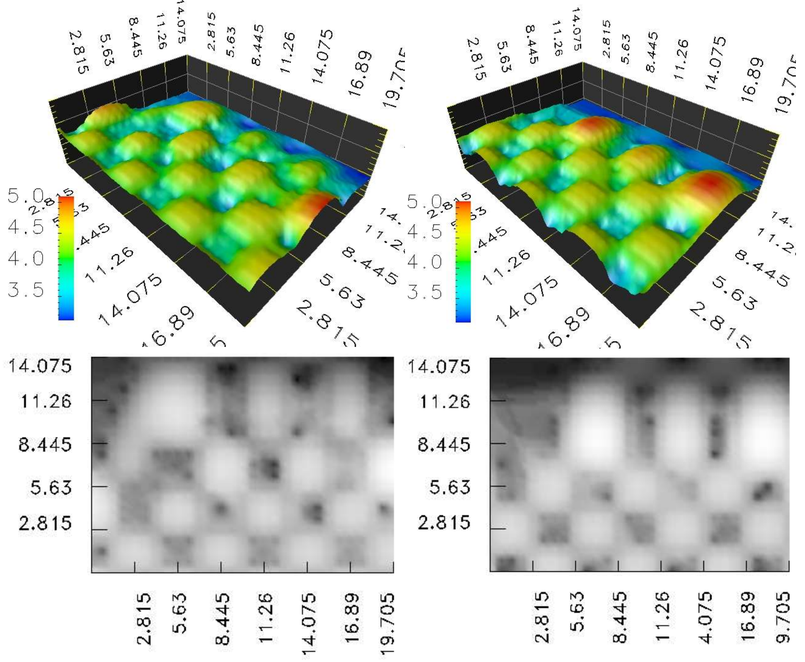

Fig. 10: Simulated results for two-atom tips perpendicular (left) and parallel (right) to the terrace. Both images are calculated at a frequency change of 140 Hz. Tick marks on pictures mark the rows of atoms; units are Å.

- Maxima no longer co-incide with atomic sites – they are shifted to interstitial positions according to the orientation of the tip-edge with respect to the surface.
- A tip with a 4-atom square down provides contrast shifted both parallel and perpendicular to the surface.

Asymmetric tips with OH impurities

- Of great interest are tips with an OH group taking the place of a Cl atom. Therefore, a symmetric OH-terminated tip was simulated, as well as asymmetric tips with an OH-Na edge down and an OH-Na-Cl edge down.

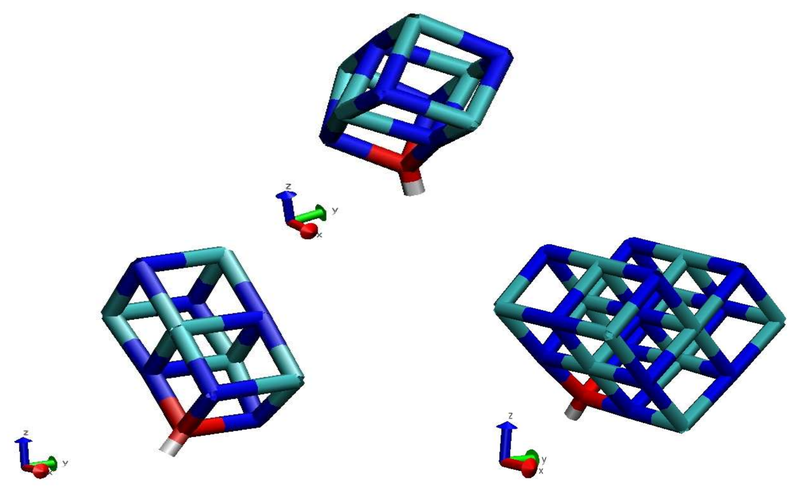

Fig. 11: The tips with one or more OH groups.

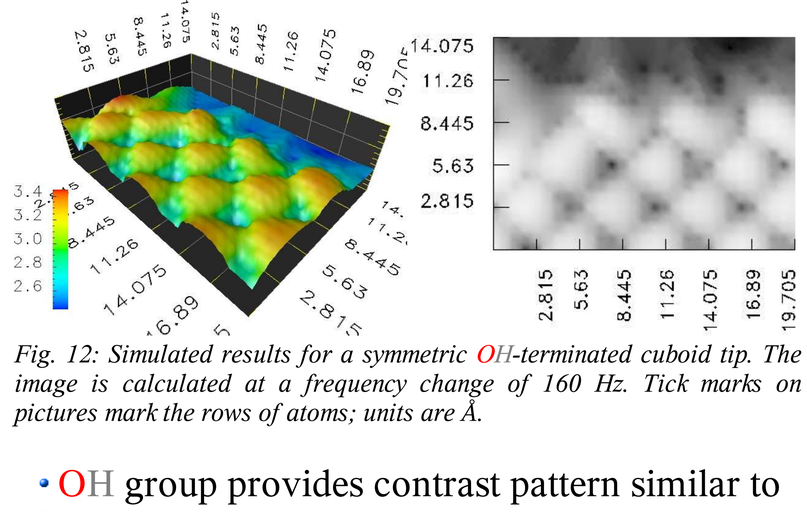

Fig. 12: Simulated results for a symmetric OH-terminated cuboid tip. The image is calculated at a frequency change of 160 Hz. Tick marks on pictures mark the rows of atoms; units are Å.

- OH group provides contrast pattern similar to Na due to positive H.
- At close approach, the influence of the higher cuboid edge produces an asymmetry in the contrast pattern.

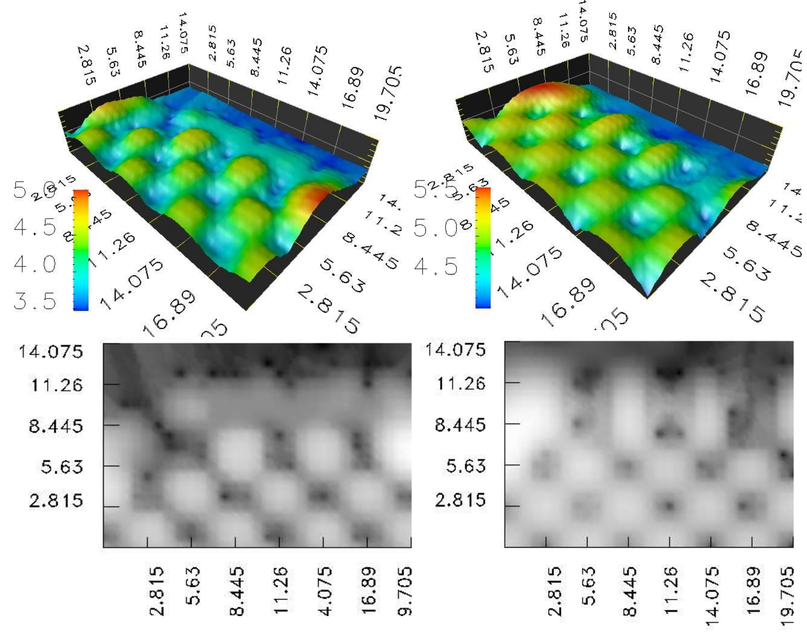

Fig. 13: Simulated results for an asymmetric OH-Na tip (left) and an asymmetric OH-Na-Cl tip with additional atoms to prevent pivoting (right). Both images are calculated at a frequency change of 140/120 Hz. Tick marks on pictures mark the rows of atoms; units are Å.

Contrast

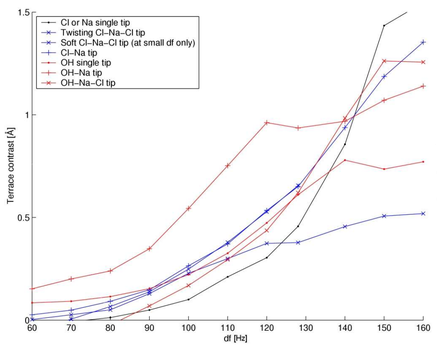

Fig. 14: Contrast on the terrace sites for different tips as a function of tip-surface distance.

- Contrast largest for ideal tip, and smallest for soft tip.
- Symmetric OH also gives small contrast, but asymmetries compensate with other ions.