Atomic and electronic structures of ternary iron arsenides $A\text{Fe}_2\text{As}_2$ (001) surfaces ($A=$Ba, Sr, or Ca)

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By the first-principles electronic structure calculations, we find that energetically the most favorable cleaved $A\text{Fe}_2\text{As}_2$ (001) surface ($A=$Ba, Sr, or Ca) is $A$-terminated with $(\sqrt{2} \times \sqrt{2})R45^\circ$ or $(1 \times 2)$ order. The $(1 \times 2)$ ordered structure yields a $(1 \times 2)$ dimerized STM image as the experiment observed. The $A$ atoms are found to diffuse on the surface with a small energy barrier so that the cleaving process may destroy the $A$ atoms ordering. At the very low temperatures this may result in an As-terminated surface with the $A$ atoms in randomly assembling. The As-terminated $\text{BaFe}_2\text{As}_2$ surface in orthorhombic phase is buckled with $(\sqrt{2} \times \sqrt{2})R45^\circ$ order, giving rise to a switchable $(\sqrt{2} \times \sqrt{2})R45^\circ$ STM pattern upon an applied bias. No any reconstruction is found for the other As-terminated surfaces. There are surface states nearby the Fermi energy found in the As-terminated and $(1 \times 2)$ $A$-terminated surfaces. A unified physical picture is thus established to help understand the cleaved $A\text{Fe}_2\text{As}_2$ (001) surfaces.