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The aging effect in topological insulator Bi2Se3 KYUNGWHA PARK, Dept. of Physics, Virginia Tech, Blacksburg, VA 24061., CHRISTOPHE DE BEULE, BART PARTOENS, Dept. of Physics, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium — Topological insulators (TIs) have attracted a lot of interest due to their topologically protected surface states, as well as exotic proximity-induced phenomena. Since the first experimental data of TIs, angle-resolved photoemission spectra (ARPES) showed that the electronic structure of the topological surface states significantly changes with time after cleavage. The origin and underlying mechanism of this aging effect are still under debate, despite its importance. Here we present our study of the evolution of the surface Dirac cone for Bi2Se3 films upon asymmetric potassium (K) adsorption, using density-functional theory and a tight-binding model. We find that the K adatoms induce short-ranged downward band bending within 2-3 nm from the surface, due to charge transfer from the K to the TI. Our findings are in contrast to earlier proposals in the literature. As the charge transfer increases, we also find that a new Dirac cone, localized slightly deeper into the TI than the original one, appears at the K-adsorbed surface, arising from strong Rashba-split conduction-band states. Our results suggest possible reinterpretations of experiments because the new Dirac cone might have been observed in ARPES measurements instead of the original one that appears just after cleavage.

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