WP12

Theoretical Methods for Condensed Matter

Part III

Tom Frömbgen

Assistants: Katharina Bauerfeind & Berenike Stahl

Submission 1: January 4, 2022

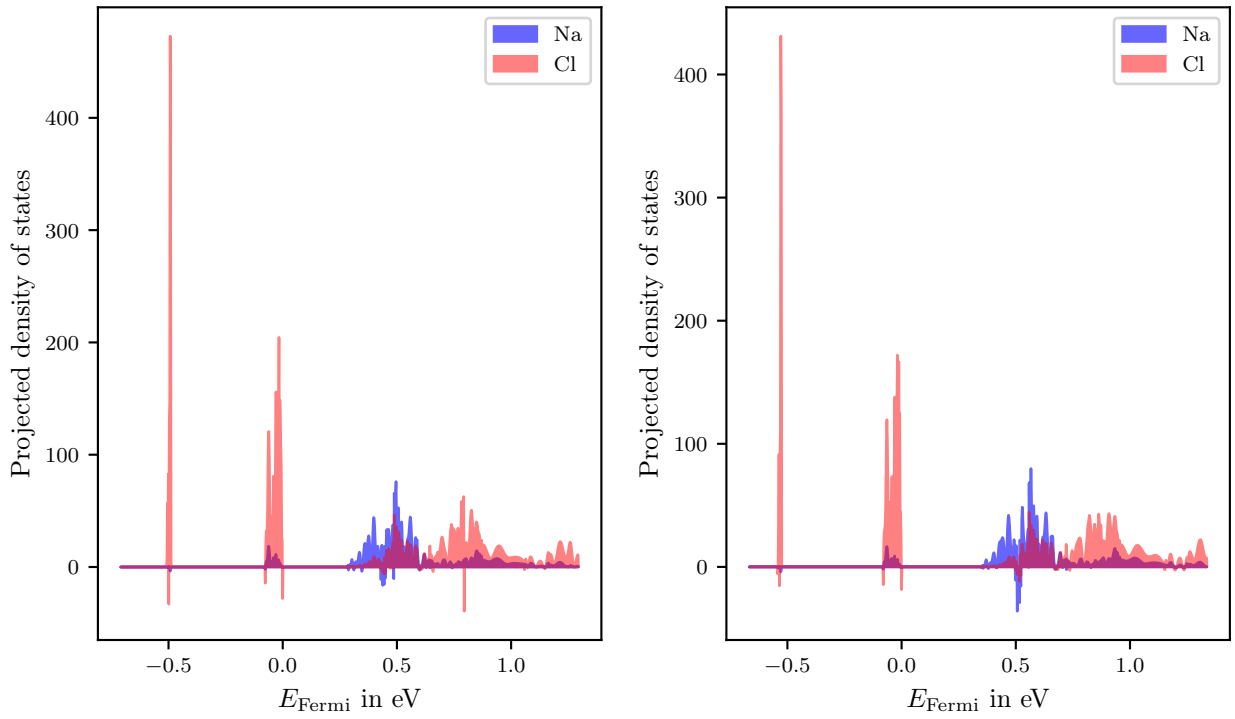

Figure 1: Projected density of states of NaCl on a PBE0/POB-TZVP level of theory with standard (left) and optimal Fock exchange fraction (right).

1 Bulk Properties

2 Calculating surfaces

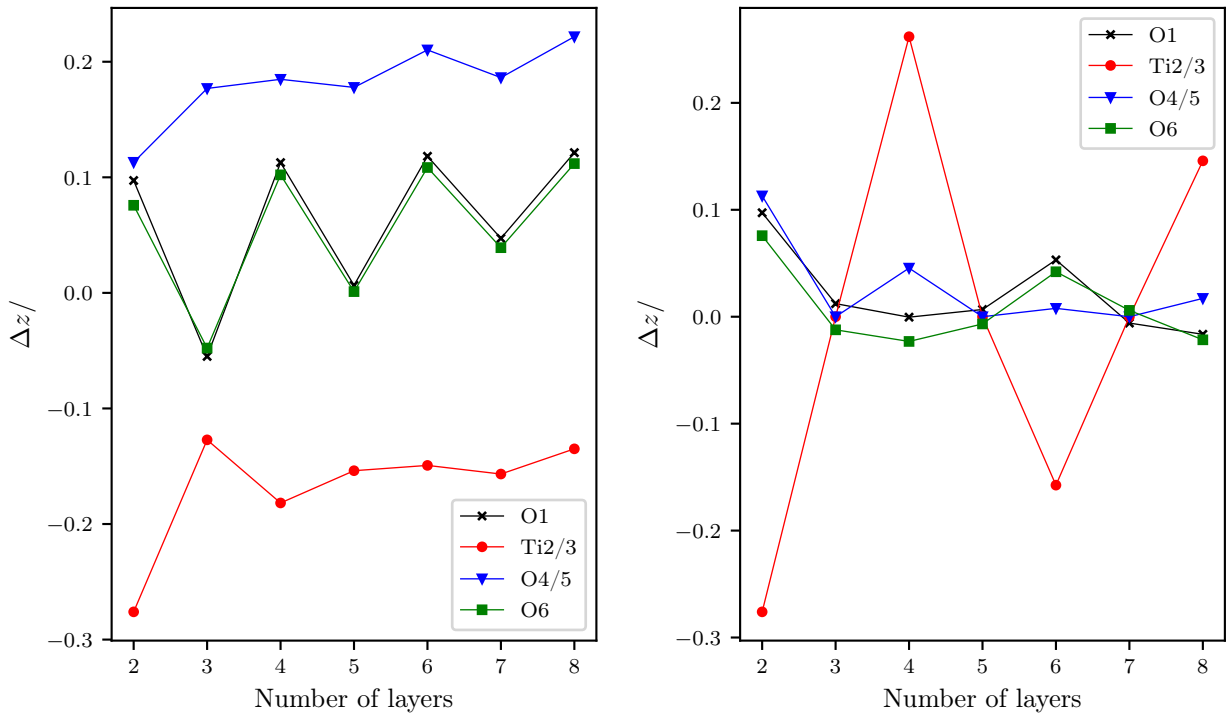

Figure 2: Relaxation of symmetry-inequivalent atoms in TiO_2 (110) surfaces of different thickness: Atoms in the topmost layer (left) are compared to bulk-like atoms in middle layers (right).

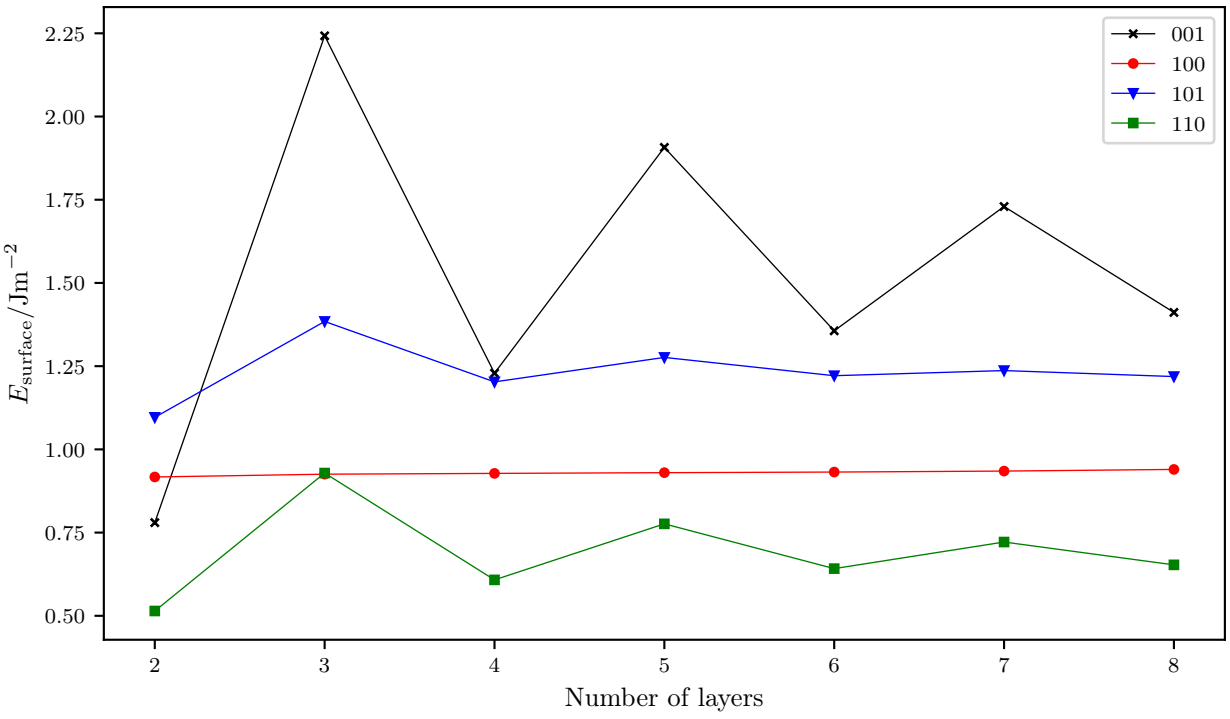

Figure 3: Calculated surface energies for different TiO_2 surfaces.