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***Ab-initio* simulations on adhesion and material transfer between contacting Al and TiN surfaces** GREGOR FELDBAUER, MICHAEL WOLLOCH, Vienna University of Technology / Austrian Center of Competence for Tribology, PETER MOHN, JOSEF REDINGER, Vienna University of Technology, ANDRAS VERNES, Vienna University of Technology / Austrian Center of Competence for Tribology — Contacts of surfaces at the atomic scale are crucial in many modern applications from analytical techniques like indentation or AFM experiments to technologies such as nano- and micro-electro-mechanical-systems (N-/M-EMS). Furthermore, detailed insights into such contacts are fundamental for a better understanding of tribological processes like wear. A series of simulations is performed within the framework of Density Functional Theory (DFT) to investigate the approaching, contact and subsequent separation of two atomically flat surfaces consisting of different materials. Aluminum (Al) and titanium-nitride (TiN) slabs have been chosen as a model system representing the interaction between a soft and a hard material. The approaching and separation is simulated by moving one slab in discrete steps and allowing for electronic and ionic relaxations after each one. The simulations reveal the influences of different surface orientations ((001), (011), (111)) and alignments of the surfaces with respect to each other on the adhesion, equilibrium distance, charge distribution and material transfer between the surfaces. Material transfer is observed for configurations where the interface is stronger than the softer material.

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