The hybrid interface between metal oxides and polymers is of great technological interest for joining, protective coating and hybrid materials. A chemical understanding of interface properties and chemistry is prerequisite for technological advancement. Computer simulations are better suited to understand these, than than experimental observation. However, existing, quantum-mechanical methods cannot handle the necessary model sizes. Techniques to couple different simulation methods to reduce computational cost are widely employed in biophysics, yet these coupling schemes cannot be directly applied to polar solids. Using density-functional based tight-binding as the QM part, existing QM/MM schemes were adapted to polar solids. QM/MM boundary treatments were adapted from biophysical applications and new methods to treat charge artifacts in polar materials were developed. The QM/MM approach saves > 90% of computer time. Adhesion of polymers on native aluminum oxide is crucial in automotive and aerospace industries. Chemisorption energies and barriers in a model adhesive were simulated. The results agree with experimental observations and explain the effect of silane adhesion promoters: more adsorption sites are favorable for them than for the other components, increasing the density of covalent bonds across the interface. The new possibility of QM/MM simulations allows inclusion of environmental effects. Initial results indicate that water at the surface strongly influences the interface.