Combined DFT and Experimental Study of Anti-Corrosion Coatings for Dental Implants

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With increasing life expectancy and improved quality of life, the demand for dental implants continues to grow. Although the current success rate of dental implant therapy exceeds 95%, certain patient groups, including diabetics, smokers, elderly patients, and oral cancer patients, may experience adverse reactions such as allergic responses, increased susceptibility to inflammation, or incomplete osseointegration, that is, the formation of a stable and functional bond between the implant and the surrounding bone tissue.

Recent research has therefore focused on surface modification of titanium implants with organic, inorganic, or biomolecular coatings to improve corrosion resistance and bioactivity, which are essential for successful osseointegration. In this study, titanium dental implants were functionalised with (*i*) alendronate, a drug commonly used in the treatment of bone diseases, and (*ii*) collagen, a structural biopolymer responsible for the mechanical stability of bone and connective tissue. The main objective of the functionalisation was to form protective coatings that increase the corrosion resistance of titanium in simulated artificial saliva, as a prerequisite for long-term biocompatibility.

The corrosion behaviour of the functionalised implants was investigated *in situ* using electrochemical impedance spectroscopy (EIS) in artificial saliva during a 7-day immersion period. Quantum-chemical calculations at the density functional theory (DFT) level enabled determination of the formation mechanisms of both coatings and revealed a key difference in their binding modes, which was reflected in the corrosion behaviour of the coated implants. The calculated Gibbs free energies for the implant–alendronate ($\Delta G^{*}_{\mathrm{INT}}$ = -13.64 kcal mol^{-1}) and implant–collagen ($\Delta G^{*}_{\mathrm{INT}}$ = -6.45 kcal mol^{-1}) interactions indicate a more spontaneous formation of the alendronate coating on the titanium surface. The DFT results also showed that the collagen coating is further stabilised by hydrogen bonding, which proved crucial for the stability of the implant in artificial saliva.

EIS measurements confirmed that the collagen coating provides about 99% protection of titanium, whereas the alendronate coating provides about 92% protection under the same conditions. The combined experimental and DFT approach was essential for interpreting the observed corrosion behaviour, which could not be fully explained based on experimental results alone.