From Surface Bioactivation to Predictive Design: Computational Perspectives on Peptide-Functionalized PEEK Interfaces

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Abstract

Implantable biomaterials play an important role in replacing or supporting damaged tissues in the human body. Among these materials, zirconia and poly(ether ether ketone) (PEEK) have attracted considerable attention for dental, maxillofacial, and orthopedic applications due to their desirable mechanical and structural properties. However, their limited surface bioactivity can restrict favorable interactions with surrounding tissues, which may ultimately affect long-term clinical performance. To overcome this limitation, surface modification strategies have been explored to enhance biological interactions while preserving the intrinsic properties of these materials.

Our experimental research has investigated surface modification strategies involving oxygen and argon plasma treatments, polydopamine, calcium and phosphate ions, and bioactive molecules, including laminin-5 and peptides containing the arginine–glycine–aspartic acid (RGD) motif. Physicochemical characterization and biological evaluations assessed their effects on cell adhesion, viability, and proliferation. Our findings demonstrated favorable cellular responses with ionic treatments, with further improvements observed following peptide incorporation. Although protein-based functionalization also showed promising results, RGD-containing peptides offer a more practical and potentially scalable alternative.

As a future direction, we propose integrating these experimental findings with computational modeling of RGD-functionalized PEEK surfaces. Building on existing physicochemical and biological data, molecular models would be developed to investigate how surface chemistry influences peptide interactions and accessibility at the molecular level. These insights could provide a foundation for developing predictive criteria to guide the rational design of bioactive PEEK interfaces.

Keywords: Biomaterials; Surface modification; PEEK; RGD peptides; Molecular modeling.