

Multiscale simulations of a peptide-zinc oxide composite

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The authors reproduced by computational means a material by using a ceramic component and a connection component for the binding of the composite inspired by Nacre, the shiny layer in seashells. The goal was to define a protein conformation that shows the highest binding capabilities to a Zinc oxide (ZnO) surface. For that, a multiscale simulation approach of coupling molecular dynamics (MD) and finite element method (FEM) simulations was established. MD simulations of a single 6-mer peptide (Fig. 1A) adsorbed on the polar ZnO(0001)-O surface were accomplished to estimate the adsorbed peptide conformations and their adsorption force parameters. The results were transferred in FE simulations with cohesive elements to define special properties of an artificial ZnO-peptide composite material. A parameter study was performed to analyze the influence of the Young's modulus of the Peptide on the mechanical properties of the material in a three point bending test. One important result in analyzing the Crack Opening Displacement (COD) (Fig. 1B) was that not only the binding capabilities of the protein should be considered as important for the fracture behavior of the nanocomposite, but also its Young's modulus.

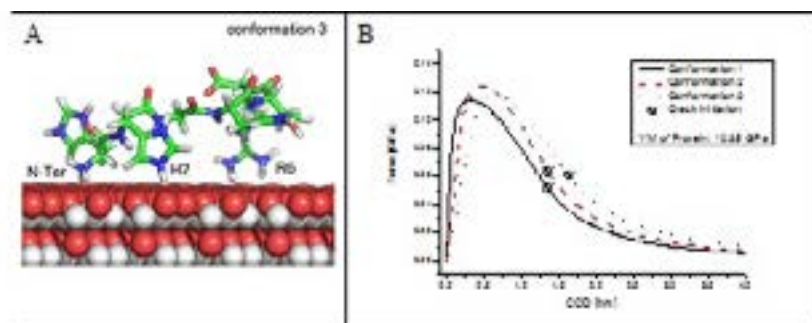


Fig. 1: A: Example conformation of the peptide on a ZnO surface. B: Comparison between different conformations of the protein [1].

Biography

Immanuel Schäfer has completed his Diploma 2009 in Biology at the University of Cologne, Germany. In 2011, he got a Master of Science in Engineering at the Carinthia University of Applied Sciences in the field of Biomimetics in Energy Systems. He is now working in the simulations of biological and bioinspired materials at the University of Stuttgart. He has published more than 5 papers in reputed journals.

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