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Prediction of Surface and pH-Specific Binding of Peptides to Metal and Oxide Nanoparticles HENDRIK HEINZ, TZU-JEN LIN, FATEME SADAT EMAMI, HADI RAMEZANI-DAKHEL, University of Akron, RAJESH NAIK, Air Force Research Laboratory, MARC KNECHT, University of Miami, CAROLE C. PERRY, Nottingham Trent University, YU HUANG, University of California-Los Angeles — The mechanism of specific peptide adsorption onto metallic and oxidic nanostructures has been elucidated in atomic resolution using novel force fields and surface models in comparison to measurements. As an example, variations in peptide adsorption on Pd and Pt nanoparticles depending on shape, size, and location of peptides on specific bounding facets are explained. Accurate computational predictions of reaction rates in C-C coupling reactions using particle models derived from HE-XRD and PDF data illustrate the utility of computational methods for the rational design of new catalysts. On oxidic nanoparticles such as silica and apatites, it is revealed how changes in pH lead to similarity scores of attracted peptides lower than 20%, supported by appropriate model surfaces and data from adsorption isotherms. The results demonstrate how new computational methods can support the design of nanoparticle carriers for drug release and the understanding of calcification mechanisms in the human body.

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