Soft Landing of Structured vs. Unstructured Peptides

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One of the primary outcomes of collisions between protonated peptides and organic self-assembled monolayer (SAM) surfaces is "Soft landing." Soft landing occurs when the peptide forms a van der Waals complex with the surface or becomes physically embedded within the surface, and was first observed experimentally by Cooks as early as 1977. This process has only recently been studied through molecular dynamics simulations; moreover, these initial soft landing trajectories focused on the relatively small peptide dialanine. Here we will present results from simulations involving much larger peptides with a focus on the differences and similarities due to secondary structure. In particular, we compare an α-helical peptide (AcA_7K) and an unstructured peptide ($AcKA_7$) in collision with a perfluorinated SAM surface. Our simulations were performed with a range of collision energies between 2.5 to 30 eV. Our preliminary findings show that the probability of soft landing does not depend on the peptide's structure, but has strong collision energy dependence. In contrast, we observe dramatic differences in the conformational entropy between the two peptides throughout the timeframe of our simulations. These findings suggest that the α-helical peptide loses it structure during the collision event.

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