



Beitrag ID: 9

Typ: **Invited Talk**

## Site-Selective Fragmentation of Peptides Induced by Swift Heavy Ions

*Freitag, 23. Januar 2026 09:50 (20 Minuten)*

The interaction of swift heavy ions (SHI) with organic matter is of high relevance for applications such as cancer therapy as well as biomaterials' development based on SHI irradiation. Furthermore, the interaction of SHI with complex molecular systems such as biomolecules is interesting from a fundamental point of view in terms of the excitation mechanisms involved and how the energy deposited in the system is coupled into the molecular degrees of freedom relevant for bond breaking. SHI-induced fragmentation of peptides serves as an ideal model system to study these processes based on the variety of functional groups and bonds in the peptide molecules.

The study of molecular fragmentation by external stimuli, however, requires an analytical tool that does not introduce fragments itself. Therefore, we make use of Desorption/Ionization induced by Neutral SO<sub>2</sub> Clusters (DINeC), an extremely soft desorption method [1], in combination with mass spectrometry (MS). DINeC-MS has proven to be an ideal tool for analyzing fragmentation processes; in particular, it was employed to investigate peptide fragmentation by SHI impact [2].

Here we ask if the interaction of SHI with peptides can lead to bond-specific and/or selective fragmentation. We find, in addition to specific fragmentation, i.e., peptide bond cleavages restricted to the peptide backbone [2], a high site-selectivity of SHI-induced fragmentation. That means that only selected peptide bonds within the amino acid sequence are efficiently broken, whereas other ones remain intact. Influence of molecular structure and ion beam properties on this surprising observation will be discussed.

[1] C. Gebhardt, et al., *Angw. Chem. Int. Ed.* 48, 4162 (2009).

[2] P. Schneider, et al., *Sci. Rep.* 12, 17975 (2022).

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**Sitzung Einordnung:** Session 3