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MERCK FROSST and the
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Chemical Dynamics Simulations of Energy Transfer, Fragmentation, and Soft-Landing in Protonated Peptide Ion Collisions with Hydrocarbon Surfaces

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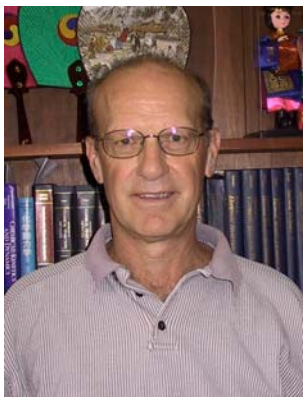
Texas Tech

Chemical dynamics simulations have been used to study energy transfer and unimolecular fragmentation in collisions of protonated peptide ions with self-assembled monolayer and diamond surfaces. Both MM and QM+MM models have been used for the simulations. The MM potential for the intermolecular interactions between the peptide ions and the surface are fit to ab initio calculations. Excellent agreement with experiments by Graham Cooks, Vicki Wysocki, and Laskin/Futrell are found from the simulations. The simulations provide an atomic-level understanding of the surface-induced dissociation (SID) experiments. Effects of peptide ion size, structure, and orientation are investigated. Surface properties, as well as the collision energy and collision angle, affect the SID dynamics. Future directions are discussed.



Professor Hase received his B.S. degree from University of Missouri-Columbia in 1967 and his Ph.D. from New Mexico State University in 1970. He was then a Post-Doctoral Fellow at New Mexico State University and University of California at Irvine before joining the faculty at Wayne State University. After 30 years at Wayne State University, he moved to Texas Tech University as a Robert A. Welch Professor of Chemistry in 2004. Professor Hase has organized many symposia and was Chair of the 2005 Gordon Research Conference on *Gaseous Ions: Structure, Energetics and Reactivity*. He is a Fellow of the American Physical Society and of the American Association for the Advancement of Science. Professor Hase's research interests lie in the theory and computer simulations of chemical dynamics, his group is actively developing *Venus, a general chemical dynamics computer program*, and he has authored or co-authored over 200 research articles and 25 book chapters and review articles in the field. He is also co-author of the books *Chemical Kinetics and Dynamics* and *Unimolecular Reaction Dynamics. Theory and Experiments*.