

Workshop D1

Interactive Exploration of Chemical Reactivity in Education

Dr. Moritz Haag, Alain Vaucher, Prof. Markus Reiher

*Lab. für Physikalische Chemie, ETH Zürich, HCI G221, Vladimir-Prelog-Weg 1-5/10, 8093 Zürich, Schweiz
moritz.haag@phys.chem.ethz.ch*

We present a virtual environment for the interactive exploration of chemical reactivity. Students can build and modify molecular structures and simultaneously study the molecule's response to the modifications. The response is transmitted to the user via a force-feedback mechanism and a structural adaptation of the unmodified parts of the molecule. Students can now directly experience the driving forces of chemical reactions and learn intuitively about the otherwise rather abstract concepts guiding chemical reactivity. For the real-time response the backend of the software runs constantly quantum mechanical calculations executed in real time. Manipulation of the structure and studying the feedback rather than calculation details are at the center of the software and allow the student to understand chemical reactivity naturally. We will demonstrate the technology at examples suitable for chemical education at high school and university level.

