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Molecular dynamics in the gas phase

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When molecules and clusters in the gas phase are excited by photons, electrons or heavier particles, a chain of events is kickstarted that may span twenty orders of magnitude in time. These processes involve, *e.g.*, ultrafast attosecond electron dynamics and its coupling to nuclear motion and molecular rearrangements occurring on picosecond timescales, which may be followed by statistical redistribution of the internal energy that leads to an intricate competition between destructive and non-destructive relaxation pathways on timescales up to minutes and beyond. Moreover, how these processes are affected by the presence of a molecular environment is largely unknown. Advancing the fundamental understanding of gas-phase molecular dynamics therefore requires complementary state-of-the art experimental and theoretical methods designed to study specific processes and to monitor them on their associated timescales in unprecedented details.

To date, laboratory tools span in size from small tailor-made table-top devices to large-scale advanced ion beam accelerators, storage rings, and novel light sources such as synchrotrons and free-electron lasers (FELs), while theoretical tools range from simple models to advanced quantum chemistry methods and approaches utilizing machine learning and artificial intelligence. Combining these tools in new and ingenious ways is key to unravelling new reaction pathways and mechanisms, and to establish their significance for a broad range of applications in, *e.g.*, astro-, radiation-, atmospheric- and material sciences. Here, examples include the formation and survival of molecules in space and their roles in star and planet formation, radiation damage of molecular systems relevant to developing new radiotherapies, and the chemistry involved in aerosol production and cloud formation.

This themed collection highlights some of the recent advances in studies of gas-phase molecular dynamics and its applications. It comprises a significant number of articles including contributions summarizing some of the work carried out by the COST Action CA18212—Molecular Dynamics in the GAS phase (MD-GAS), supported by COST (European Cooperation in Science and Technology), **https://www.cost.eu/actions/CA18212/**. This demonstrates the success of this highly interdisciplinary network, which has been running between the years 2019–2024 and now contains more than 400 researchers from 35 countries across the globe.

We, the guest editors, would like to thank all authors for contributing high-quality articles and to all participants of the MD-GAS COST Action. Furthermore, we would like to thank the PCCP editorial staff for their invaluable support and excellent guidance from day one to the completion of this themed collection. We hope that it will attract a broad range of readers from the fields of fundamental physics, chemical physics, and physical chemistry to those from more applied ones, such as astrophysics and -chemistry, astronomy, atmospheric science and radiation science.

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