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Atomistic simulations of reactive processes in the gas- and condensed-phase

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This review focuses on force-field-based approaches to investigate – through computer simulations – reactive processes in chemical and biological systems. Both, reactions in the gas-phase and in condensed-phase environments are discussed and opportunities and the potential for further developments are pointed out. Where available, results are compared with alternative methods and the advantages and drawbacks of the methods are compared. Particular applications include vibrationally and electronically induced (photo)dissociation of small molecules, proton transfer in the gas- and condensed phase and ligand un- and re-binding in proteins.
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