Simple Quantum Chemistry for Complex Systems and Processes

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Two topics from our recent theoretical research will be presented:
1. Computation of electron-impact mass spectra (EI-MS) based on a combination of fast quantum chemical methods, molecular dynamics, and stochastic preparation of 'hot' primary ions. The approach considers basic elementary processes with minor empiricism, employs realistic potential energy surfaces computed 'on-the-fly', is 'black-box' and provides decent spectra accompanied by detailed information of corresponding decomposition and reaction mechanisms. For the first time it enables the routine calculation of chemically important mass spectrometric data[1].
2. Automatic generation of a general inter- and intramolecular force-field from dispersion corrected DFT. The method (termed QMDFF) can be applied without specific fitting to any molecular system (including metal complexes), allows smooth dissociation of a molecule into atoms or fragments, and yields consistent intra- and intermolecular forcespproaching DFT quality [2]. It has recently made "reactive" which will be discussed briefly [3].

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3. Hartke, B.; Grimme, S. *Phys. Chem. Chem. Phys.* 2015, *17*, 16715-16718.