Efficient density-functional theory force evaluation for large molecular systems - recent developments in DALTON

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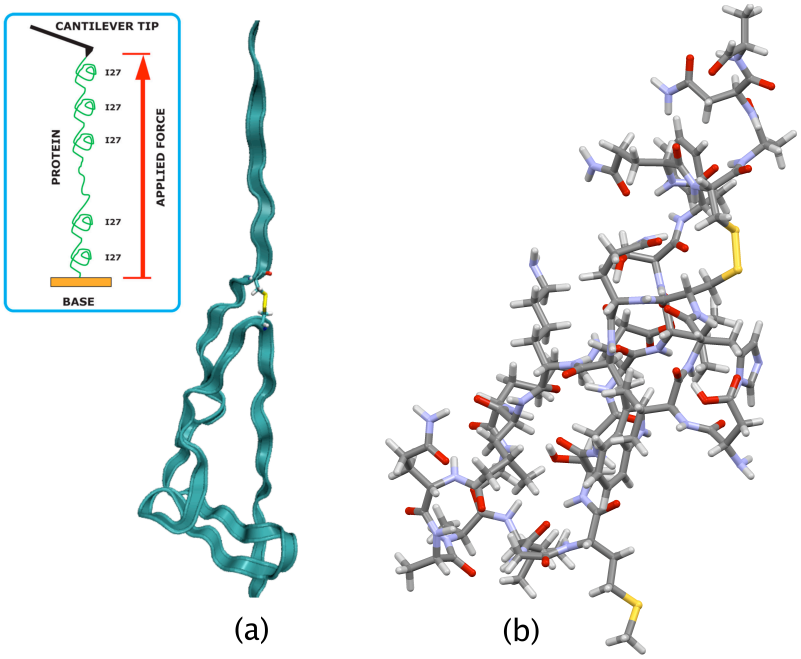
In this talk we report recent developments in DALTON for the efficient evaluation of density-functional theory forces. The new developments are based upon a novel integral evaluation scheme[1] and density-fitting and linear-scaling technology[2]. The efficiency and linear complexity of the molecular-force evaluation is demonstrated by sample calculations on molecular systems contaning up to 642 atoms, and for the geometry optimization of a few selected large systems contaning up to 392 atoms.



Literature:
[1] S. Reine, E. Tellgren and T. Helgaker, Phys. Chem. Chem. Phys. **9**, 4771 (2007). [2] S. Reine, A. Krapp, M. F. Iozzi, V. Bakken, T. Helgaker, F. Pawłowski, P. Sałek, J. Chem. Phys. **133**, 044102 (2010).