Libxc – a library of exchange and correlation functionals

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LIBXC [1, 2] is a library of exchange-correlation functionals for density-functional theory. We are concerned with semi-local functionals (or the semi-local part of hybrid functionals), namely local-density approximations, generalized-gradient approximations, and meta-generalized-gradient approximations.
Currently we include more than 400 functionals for the exchange, correlation, and the kinetic energy, spanning more than 50 years of research. Moreover, LIBXC is by now included in more than 20 codes, not only from the atomic, molecular, and solid-state physics, but also from the quantum chemistry community.

References

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[2] "Libxc: a library of exchange and correlation functionals for density functional theory", M.A.L. Marques, M.J.T. Oliveira, and T. Burnus, Comput. Phys. Commun. **183**, 2272-2281 (2012)