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Enabling accurate, fast, and out-of-the-box simulations of organic compounds with artificial intelligence

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We use AI to enable fast and accurate calculations of the quantum chemical properties of organic molecules, which were not achievable with traditional methods. The most powerful of our methods is AIQM1 which is both more accurate and faster than popular B3LYP/6-31G* and similar DFT methods.[1] AIQM1 can be used to perform geometry optimizations (often with sub-picometer accuracy)[1] and MD as well as calculate heats of formation obtained with AIQM1 with chemical accuracy[2] and uncertainty estimates.[2] AIQM1 can be used as a robust approach for locating TSs with reasonable accuracy.[3] AIQM1 was applied for uncovering the nature of real-life ground- and excited-state chemistry of polyparaphenylene nanolassos.[4]

Our AI methods are available in an open-source MLatom package and calculations can be performed on a XACS cloud computing platform (http://XACScloud.com). MLatom also supports a wide range of other simulations (http://MLatom.com/manual), including accelerated computation of one- and two-photon absorption spectra[5-6].

References:

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