

On the Structure and Geometry of Biomolecular Binding Motifs (Hydrogen-Bonding, Stacking, X-H $\cdots\pi$): WFT and DFT Calculations [*Journal of Chemical Theory and Computation* 2010, 6, 66–80. DOI: 10.1021/ct900376r]. Kevin E. Riley,* Michal Pitoňák, Jiř Cerný, and Pavel Hobza*

It is stated in the article that, “[T]he incorrect long-range behavior of the M06-2X functional is due to the fact that the dispersion energy was covered by reparameterization of the exchange functional and not by the correlation one.” This statement is incorrect; this functional describes dispersion-like interactions using the correlation (and not the exchange) term. The proper explanation for the poor behavior of this functional at long-range (in the nonoverlap region) lies in the functional’s inherently local nature.

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