Abstract Submitted
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Pair-Wise and Many-Body Dispersive Interactions Coupled to an Optimally Tuned Range-Separated Hybrid Functional LEEOR KRONIK, PIYUSH AGRAWAL, Weizmann Institute of Science, ALEXANDRE TKATCHENKO, Fritz-Haber-Institute, Berlin — We propose a nonempirical, pair-wise or many-body dispersion-corrected, optimally tuned range-separated hybrid functional. This functional retains the advantages of the optimal-tuning approach in the prediction of the electronic structure. At the same time, it gains accuracy in the prediction of binding energies for dispersively bound systems, as demonstrated on the S22 and S66 benchmark sets of weakly bound dimers.

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