

Development and implementation of D4: A charge dependent molecular dispersion coefficient model

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The semiclassical D3 model presented in 2010 is one of the most widely used scheme to describe long-range London dispersion interactions with about 3800 citations (web of science) during the last six years. Apart from its accuracy (dispersion coefficients are, on average, accurate to around 5%) the major advantage of the D3 approach relies in its computational efficiency. The presented work developed a charge dependent model that is able to combine the computational efficiency of D3 with electronic structure information. Atomic partial charges are calculated self-consistently using an extended tight-binding Hamiltonian available for the whole periodic table. Those data are used as descriptors to scale reference TD-DFT polarizabilities at imaginary frequencies to calculate charge dependent dispersion coefficients via numerical on-the-fly Casimir-Polder integration. Statistical data regarding the accuracy and efficiency of the charge dependent approach are presented. A stand-alone program to calculate charge dependent dispersion coefficients as well as charge dependent polarizabilities for given molecular coordinates can be downloaded free of charge from our website.