

Abstract Submitted  
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**Short-range Cut-Off of the Summed-Up van der Waals Series<sup>1</sup>**

ABHIRUP PATRA, JOHN P. PERDEW, Temple University — van der Waals interactions are important in typical van der Waals-bound systems such as noble-gas, hydrocarbon, alkali and alkaline-earth dimers. The summed-up van der Waals series [1,2] works well and gives an accurate result at large separation between two atoms. But it has a strong singularity at short non-zero separation, where the two atoms touch. In this work we remove that singularity with a reasonable and physical choice of the cut-off distance. Only one fitting parameter has been introduced for the short-range cut off. The parameter in our model has been optimized for each system, and a system-averaged value has been used to get the final binding energy curves. When this correction is added to the binding energy curve from the semilocal density functional meta-GGA-MS2, we get vdW- corrected binding energy curve. These curves are compared with the results of other vdW-corrected methods such as PBE-D2 and vdW-DF2 .Binding energy curves are in reasonable agreement with those from experiment. These curves also predict reasonably good equilibrium bond length. [1] J.P. Perdew, A. Ruzsinszky, J. Sun and S. Glindmeyer, Physical Review A 86, 062714 (2012). [2] A. Ruzsinszky, J.P. Perdew, J. Tao, and G.I. Csonka Physical Review Letters 109, 233203 (2012).

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