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Higher-order van der Waals coefficients from static multipole polarizability[1] JIANMIN TAO, JOHN PERDEW, ADRIENN RUZSINSZKY, Tulane University — van der Waals interaction is a long-range nonlocal correlation arising from instantaneous charge fluctuations on each fragment. Though very weak, it considerably affects the properties of molecules and solids. Evaluation of van der Waals coefficients is of strong current interest. In this work, we have derived a general expression for these coefficients in terms of static multipole polarizability only. Applications of the present theory to atom as well as molecular pair interactions have been made.

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