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Efficient van der Waals density functional interactions[1] JOSE M. SOLER, GUILLERMO ROMAN-PEREZ, Univ. Autonoma de Madrid — The LDA and GGA functionals are the non empirical methods of choice for large system calculations, but they cannot describe nonlocal dispersion forces. This limits severly their application to many systems of large interest, like molecular solids and liquids, physisorbed molecules, and interactions between biological molecules. Several schemes have been proposed to add ad-hoc atom-atom or atom-electron potentials. But dispersion is an electron-electron correlation effect, that must be described by an appropriate electron density functional, such as that proposed by Dion et al (PRL 92, 246401 (2004)). It is a true universal and general-purpose DFT functional that describes semiquantitatively the week dispersion interactions, without compromising the accuracy of the best GGA functionals for stronger bonds. Its direct evaluation for large molecular systems is very expensive, however, because it requires a double integral in real space. We present a new implementation that avoids this N^2 scaling by applying Fourier convolution techniques to an accurately interpolated kernel. The resulting method scales as $N \log N$ and it allows to perform vdW-DFT simulations of essentially any system that can be simulated with GGA.

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