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A Qbox Implementation of van der Waals Density Functionals with Applications[1] JUN WU, Graduate Group in Applied Science, University of California Davis, Davis CA 95616, FRANCOIS GYGI, Department of Computer Science, University of California Davis, Davis CA 95616 — We present an implementation of the non-local van der Waals correlation functional proposed by Dion et al. [1] in the Qbox code [2]. We develop a simple approach to remove the logarithmic singularity in the kernel function, and derive the non-local potential needed for self-consistent calculations of energies, ionic forces and stress for simulations in arbitrary-shaped unit cells. We compare the performance of five different van der Waals functionals in applications to the benzene-water dimer, the benzene crystal and other organic molecular crystals.

[1] M. Dion et al. Phys. Rev. Lett. 92, 246401 (2004)
[2] http://eslab.ucdavis.edu/software/qbox

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