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A Scalable Implementation of Van der Waals Density Functionals[1] JUN WU, FRANCOIS GYGI, University of California Davis — Recently developed Van der Waals density functionals[1] offer the promise to account for weak intermolecular interactions that are not described accurately by local exchange-correlation density functionals. In spite of recent progress [2], the computational cost of such calculations remains high. We present a scalable parallel implementation of the functional proposed by Dion et al.[1]. The method is implemented in the Qbox first-principles simulation code (http://eslab.ucdavis.edu/software/qbox). Application to large molecular systems will be presented.

[1] M. Dion et al. Phys. Rev. Lett. 92, 246401 (2004).
[2] G. Roman-Perez and J. M. Soler, Phys. Rev. Lett. 103, 096102 (2009).

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Francois Gygi
University of California Davis

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