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Efficient van der Waals energy calculations via a continuum mechanics approach TIM GOULD, JOHN F. DOBSON, Qld Micro- and Nanotechnology Centre, Griffith University, Nathan, Qld 4111, Australia, ILYA V. TOKATLY, IKERBASQUE, Basque Foundation for Science, E-48011, Bilbao, Spain
— Recent developments in continuum mechanics (CM) [Tao *et al*, PRL**103**,086401] enable the calculation of density response functions from groundstate properties only. Using the direct Random Phase Approximation (dRPA) we develop this CM approach into a third-rung van der Waals energy functional, which we dub the CM-dRPA. The functional requires as input the groundstate Kohn-Sham potential $V^{\rm KS}(\vec{r})$, density $n^0(\vec{r})$ and a kinetic stress tensor $\mathrm{T}^0(\vec{r})$ defined via $T^0_{\mu\nu} = Re\sum_{i\rm occ}\psi^*_{i,\mu}\psi_{i,\nu} - n^0_{,\mu,\nu}/4$ where ψ_i is an orbital. We present efficient algorithmic schemes for its evaluation in bulk and molecular systems using the full eigen-solutions of the bare CM equation and a second, simpler evaluation to find the interacting eigenvalues. These eigen-solutions are then used to calculate the correlation energy via a simple summation. The CM-dRPA is *significantly* faster than a full dRPA calculation in systems with many electrons. We then apply the CM-dRPA functional to metallic, slab-like 2D-homogeneous jellium systems and periodic solids, with good results for vdW dispersion. In the metallic case most efficient vdW functionals would fail qualitatively.

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