A new 3rd-rung correlation energy functional based on quantum continuum mechanics: application to van der Waals forces.

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The linear Quantum Continuum Mechanics theory [1,2] is used to approximate electronic response and hence to obtain approximately the RPA correlation energy of interacting inhomogeneous many-electron systems. The resulting correlation energy expression is an implicit energy functional that uses as inputs the Kohn-Sham groundstate density and also a "new density", the Kohn-Sham kinetic stress tensor T_0(r) that can be evaluated entirely from the occupied groundstate Kohn-Sham orbitals and their space derivatives. It is therefore an (implicit) 3rd rung energy functional. This approach has been tested so far on the anomalous van der Waals (vdW) interaction between overlapping and non-overlapping thin jellium metal slabs [3], and on the lattice spacing of some 3D crystals . Currently popular vdW energy functionals do not capture the D^(-5/2) power law for thin metallic slabs, in contrast to the present functional.

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