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【118】All-electron benchmark results with nonlocal van der Waals functionals

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The method of Roman-Perez and Soler [Phys. Rev. B 103, 096102 (2009)], which allows for a fast implementation of the nonlocal van der Waals (vdW) functionals, has contributed in making the vdW functionals popular. However, the Roman-Perez-Soler method relies on a plane-wave expansion of the electron density, therefore it can not be applied to all-electron densities for which an unaffordable number of plane waves would be required for an accurate expansion. We present the results for the lattice constant and binding energy of solids that were obtained by applying a smoothing procedure to the all-electron densities. It is shown that the results agree very well with those from the literature.

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