Local response dispersion method in periodic systems: Implementation in the package based on a plane-wave basis set

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A number of dispersion correction methods have been developed to make density functional theory (DFT) applicable to noncovalent interactions. Our group has proposed and extended the local response dispersion (LRD) method,[1-5] which evaluates density-dependent dispersion coefficients using the result of DFT calculation. The LRD method was implemented in the program based on Gaussian basis functions. The availability of the LRD method was investigated not only for conventional hydrogen-bonded and dispersion-dominated molecular complexes but also for open-shell systems[4] and excited states.[5] Since the implementation in the program based on a plane-wave basis set was not reported, this study implements the LRD method into Quantum Espresso and examines the accuracy of the LRD method for periodic systems.

As a primary application, we optimized lattice parameters and cohesive energies of urea. Here, the LRD method is combined with the revised Perdew-Burke-Ernzerhof (revPBE) functional.[6] According to Table 1, significant improvements in structure and energetics are achieved. Numerical results of other periodic systems and details of the implementation will be explained in the poster session.

Table 1. Optimized lattice parameters and cohesive energies of urea. Differences from the experiments are shown in parentheses.

	revPBE		revPBE+LRD		Expt.
Lattice parameter					
a (Å)	6.055	(0.490)	5.638	(0.073)	5.565[7]
c (Å)	4.768	(0.084)	4.722	(0.038)	4.684[7]
V (Å^3)	174.8	(29.7)	150.1	(5.1)	145.1[7]
Cohesive energy (kcal/mol)	13.49	(-9.75)	23.26	(0.02)	23.24[8]

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