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Non-local exchange-correlation term implemented into the density functional theory YOUKY ONO, Center for Frontier Science, Chiba university, KOICHI KUSAKABE, Graduate School of Engineering Science, Osaka university, TAKASHI NAKAYAMA, Faculty of Science, Chiba University — The local density approximation (LDA) has serious limitation that this approximation cannot estimate the long-ranged (non-local) exchange-correlation interaction, as typified by the van der Waals (vdW) interaction. In this study we develop a method to calculate the vdW interaction based on the LDA together within the plasmon-pole approximation [1]. The computation code is developed as one of a module program of an existing first principle calculation package. Usefulness and efficiency of the method are confirmed by calculating the interaction energy of simple periodic systems. This method never relies on external parameters and/or on asymptotic model functions, and thus being applicable to any isolated 3 dimensional structures. [1] PRL **96**, 073201 (2006), PRB **62**, 6997 (2000), PRL **92**, 246401 (2004).

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