Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Stress and Vibrational Properties of non-local van der Waals exchange-correlation functionals RICCARDO SABATINI, International School for Advanced Studies (SISSA), via Bonomea 265, 34136 Trieste, Italy, STEFANO DE GIRONCOLI, International School for Advanced Studies (SISSA) and CNR-IOM DEMOCRITOS Simulation Center, via Bonomea 265, 34136 Trieste, Italy — Van der Waals interaction is an essential component in the description of soft matter and plays an important role in many other systems, from adsorbates to water interaction. Within the framework of Density Functional Theory in the last years a great effort has been made to overcome the limitations of LDA or GGA functionals, and a new class of non-local functionals is now filling the gap giving interesting results. We present here several new improvements in this field, and some selected applications. In particular, i) we worked out the theoretical formalism needed to define both the stress tensor and the phonon vibrations associated to the non-local functional form proposed by Dion[1], and ii) we developed and implemented in the Quantum ESPRESSO simulation package a new functional inspired by the work of Vydrov and Van Voorhis[2], simple to compute efficiently in plane wave approach and with great performances on the S22 set. Finally we present some results obtained on aminoacid crystal and other simple molecules where these new tools are benchmarked and compared with experimental results and other theoretical approaches.

[1] M. Dion, B. I. Lundqvist et al., Phys. Rev. Lett. 92, 246401 (2004);
[2] Oleg A. Vydrov and Troy Van Voorhis , Phys. Rev. Lett. 103, 06300

Riccardo Sabatini
International School for Advanced Studies (SISSA),
via Bonomea 265, 34136 Trieste, Italy

Date submitted: 29 Nov 2011 Electronic form version 1.4