Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Range-separated approach to the RPA correlation applied to van der Waals bond and to diffusion of defects FABIEN BRUNEVAL, CEA — The Random Phase Approximation (RPA) is a promising approximation to the exchange-correlation energy of Density Functional Theory (DFT), since it contains the van der Waals (vdW) interaction and yields a potential with the correct band gap. However, its calculation is computationally very demanding. We apply a range separation concept [1] to RPA and demonstrate how it drastically speeds up the calculations without loss of accuracy. The scheme is succesfully applied to a layered system subjected to weak vdW attraction and to address the controversy of the self-diffusion in silicon [2]. We calculate the formation and migration energies of self-interstitials and vacancies taking into account atomic relaxations. The obtained activation energies deviate significantly from the earlier calculations that were affected by the band gap problem and challenge some of the experimental interpretations [3]: the diffusion of vacancies and interstitials have almost the same activation energy.

[1] J. Toulouse, F. Colonna, and A. Savin, Phys. Rev. A **70**, 062505 (2004).
[2] F. Bruneval, Phys. Rev. Lett. **108**, 256403 (2012).
[3] H. Bracht, E. E. Haller, and R. Clark-Phelps, Phys. Rev. Lett. **81**, 393 (1998).

Fabien Bruneval
CEA

Date submitted: 23 Oct 2012 Electronic form version 1.4