s2.m2.o5 Electron correlation effects through analysis of electron densities. S. Ragot, P.J. Becker, J.M. Gillet. *SPMS, Ecole Centrale Paris, Grande Voie des Vignes, 92295 CHATENAY MALABRY, France.*
Keywords: momentum density, electron correlation.

Electron correlation, and its effect on cohesive properties, has been a subject of constant research during last decades. On the experimental side: electron momentum density can be accessed and analyzed through Compton scattering[1], and the electron pair density function can be in principle observed through total x-ray scattering[2]. Owing to these experimental possibilities, we have investigated simple models for the two-particle density matrix (2DM).

After a discussion of the general properties of the 2DM, we concentrate onto two main applications.

1. Local correlation. Comparing experimental and computed SCF momentum densities in MgO and LiH crystals, a significant isotropic discrepancy occurs[3]. This effect remains with different experiments, and within different basis-set calculations. We show how correlations can be invoked to explain some of these differences. These observations are closely related to the shape of the coulomb hole.

2.Intermolecular forces. Correlation plays an important role in the cohesion of molecular solids. We propose a modelisation of the influence of Van der Waals (VDW) forces onto charge and momentum densities. We show that VDW effects, though quite small, should be more pronounced in momentum space than real space.

Notes

[1] B. Williams (1977). Compton Scattering. McGraw-Hill
[2] Calzuola G., Petrillo C., Sacchetti F. (1999) Phys. Rev. A60, 4135
[3] Fluteaux C. (1999) thesis