Efficient algorithms for Hirshfeld-I charges

Kati Finzel[1], Angel M. Pendas[2], Evelio Francisco[2]

1. On leave from Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, now at Linköpings Universitetet, IFM, Fysikhuset, 58183 Linköping, Sweden
2. Dpto. Química Física y Analítica. Universidad de Oviedo. Spain

A new viewpoint on iterative Hirshfeld charges is presented, whereby the atomic populations obtained from such a scheme are interpreted as such populations which reproduce themselves. This requirement can be expressed analytically rather than being understood as the result of an iterative procedure. Based on that analytical expression much faster algorithms for Hirshfeld-I charges have been developed. In addition new atomic reference densities for the Hirshfeld-I procedure are presented. The proposed reference densities are N-representable, display proper atomic shell structure and can be computed for any charged species.