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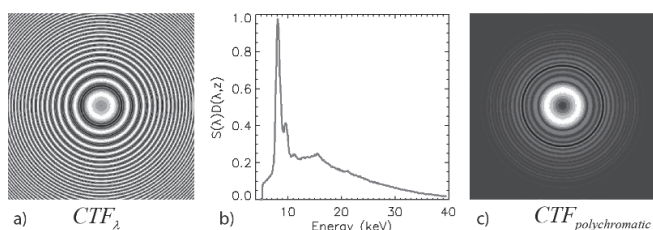
Quantitative phase imaging with polychromatic sources

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In most laboratories, X-ray sources are polychromatic. To date, X-ray absorption contrast imaging with polychromatic sources has produced good qualitative results when it is used for high absorbing objects. However, the application of the absorption based technique to weakly absorbing objects remains limited.

Phase contrast imaging has been widely recognized as a unique tool to study weakly absorbing objects [1], [2], [3]. A phase retrieval algorithm based on the so-called Contrast Transfer Function (CTF) approach [4] has been demonstrated to quantitatively reconstruct the thickness of weakly absorbing homogeneous samples using monochromatic sources. The technique can be applied to propagation distances ranging from the near field to the holographic regions.

In this work we propose an extension of the CTF algorithm to polychromatic sources [3]. Principles and simulated results of the new technique will be presented. We will discuss quantitative experimental results for homogeneous samples using (a) synchrotron radiations with a significant harmonic content; and (b) a laboratory X-ray source. The experimental results indicate highly potential applications of the technique to quantitative studies of both 2D and 3D samples.



[1] S.W. Wilkins, T.E. Gureyev, D. Gao, A. Pogany, A.W. Stevenson, *Nature* **1996**, 384, 335. [2] B. Arhatari, K. Hannah, E. Balaur, A. Peele, *Opt. Express* **2008**, 16, 19950. [3] M.B. Luu, B.D. Arhatari, C.Q. Tran, E. Balaur, B.T. Pham, N.T. Vo, B. Chen, C.T. Putkunz, N. Kirby, S. Mudie, A.G. Peele, *Opt. Express* **2011**, 19, 8127. [4] L. Turner, B. Dhal, J. Hayes, A. Mancuso, K. Nugent, D. Paterson, R. Scholten, C. Tran, A. Peele, *Opt. Express* **2004**, 12, 2960.

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An account on multicenter bonding and its relationship with aromaticity

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There has been renewed interest in the calculation of different indices based on the electron density matrices to account for multicenter bonding [1-6]. Some of these quantities have also been used as aromaticity indices, providing very good results as compared to other aromaticity indicators [7], [8]. Multicenter indices are thus perfect

candidates to account for aromaticity from the electron delocalization perspective. The general formula for the calculation of the multicenter index involves the very intuitive n -order central moment of the electron population used in probability theory [9], [10]:

Unfortunately, the calculation of this quantity is not trivial, especially in correlated methods for which the computation of the n -density matrix is necessary. In this talk we review the concept of multicenter bonding and its application to aromaticity. First we present I_{ring} [1], MCI [2] and their recently introduced normalized variants, I_{NG} and I_{NB} [3]. We analyze the different formulations suggested in the literature, either in terms of the corresponding n -density matrix or its simplified version in terms of the first-order density matrix. An analysis of the differences between these approaches is performed and we suggest new formulae, which approximate the n -density matrices in different ways.

[1] M. Giambiagi, M.S. d. Giambiagi, C.D. dos Santos Silva, A.P. da Figueiredo, *Phys. Chem. Chem. Phys.* **2000**, 2, 3381. [2] P. Bultinck, R. Ponec, S. Van Damme, *J. Phys. Org. Chem.* **2005**, 18, 706. [3] J. Cioslowski, E. Matito, M. Solà, *J. Phys. Chem. A* **2007**, 111, 6521. [4] A.M. Pendás, E. Francisco, M.A. Blanco, *Phys. Chem. Chem. Phys.* **2007**, 9, 1087. [5] A. M. Pendás, E. Francisco, M.A. Blanco, *J. Chem. Phys.* **2007**, 127, 144103. [6] R. Ponec, I. Mayer, *J. Phys. Chem. A* **1997**, 101, 1738. [7] F. Feixas, E. Matito, J. Poater, M. Solà, *J. Comput. Chem.* **2008**, 29, 1543. [8] F. Feixas, J.O.C. Jiménez-Halla, E. Matito, J. Poater, M. Solà, *J. Chem. Theory Comput.* **2010**, 6, 1118. [9] M. Giambiagi, M. Giambiagi, K. Mundim, *Struct. Chem.* **1990**, 1, 423. [10] E. Francisco, A.M. Pendás, M. A. Blanco, *J. Chem. Phys.* **2007**, 126, 094102.

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The hirshfeld-i method: atoms in molecules and chemical bonding perspective

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The Hirshfeld method for the atom in the molecule (AIM) was born from crystallography and relies on the use of a so-called promolecule [1]. The promolecule is composed of all atoms in their respective locations in the molecule and a promolecular density is obtained as the sum of all isolated atomic densities. At every point in space, the share of an (isolated) atom in the promolecular density can be easily computed via their ratio and the key element of the Hirshfeld method is that this ratio is then used to extract an AIM density from the molecular electron density. That is:

$$D(A_1, K, A_n) \sim \left\langle \left(\hat{N} - \bar{N} \right)^n \right\rangle_{A_1, K, A_n}$$

Unfortunately, the results of Hirshfeld analysis depend heavily on the isolated atom states used to compute the AIM weight functions. In the improved Hirshfeld-I method, the Hirshfeld process is repeated until self consistency is reached. In other words: the charge on the AIM and the isolated atom are the same. In this presentation the information theoretic context of Hirshfeld-I is sketched, performance of the method compared to regular Hirshfeld analysis discussed, its impact on the nature of atom condensed Fukui functions described, and its use for good quality monopole approximation electrostatic potentials is shown [2-6].

Electron delocalization indices, as obtained using the Hirshfeld-I method, are described [7] and the excellent Hirshfeld-I AIM charge