Local self-interaction correction in LSMS. MARKUS EISENBACH,
G. M. STOCKS, ORNL — While local density approximation (LDA) calculations
have proven to be exceptionally successful for performing first principles calcula-
tions materials generally thought of as being strongly correlated (e.g. transition
metal oxides) are poorly described. However, for many of these systems, it is now
clear that an important factor in this failure is the self-interaction error that results
in an unphysical Coulomb interaction of an electron with itself. This error can be
readily accounted for by use of self-interaction corrected (SIC) LDA [1,2]. Here we
report on our implementation of the recently developed local SIC (L-SIC) formula-
tion developed by Lüders et al. [3] and which is particularly well suited to multiple
scattering theory based electronic structure methods. Here we will describe the
implementation of L-SIC in our order-N locally self-consistent multiple scattering
(LSMS) code as well results for example applications f-electron and TMO systems.
1. J. P. Perdew & A. Zunger, PRB 23, 5048 (1981). 2. Z. Szotek et al., J. Phys.:CM
16, S5587-S5600 (2004). 3. M. Lüders et al., PRB 71 205109 (2005). This research is
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