

# PERIODIC DENSITY FITTED LOCAL CIS

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A new density fitted local CIS method for periodic systems as implemented in the CRYSCOR [1] code is presented. In its current implementation it can describe Frenkel and intermediate-ranged  $\Gamma$ -point excitons in one-dimensional periodic systems. The procedure is partly performed in direct and partly in reciprocal space. The periodic CIS method is able to capture the electron-hole-interaction and constitutes a first step towards correlated optical band gaps in periodic systems.

## Literature:

[1] M. Schütz, D. Usvyat, M. Lorenz, C. Pisani, L. Maschio, S. Casassa, M. Halo, *Accurate Condensed-Phase Quantum Chemistry*, will be published in May 2010.