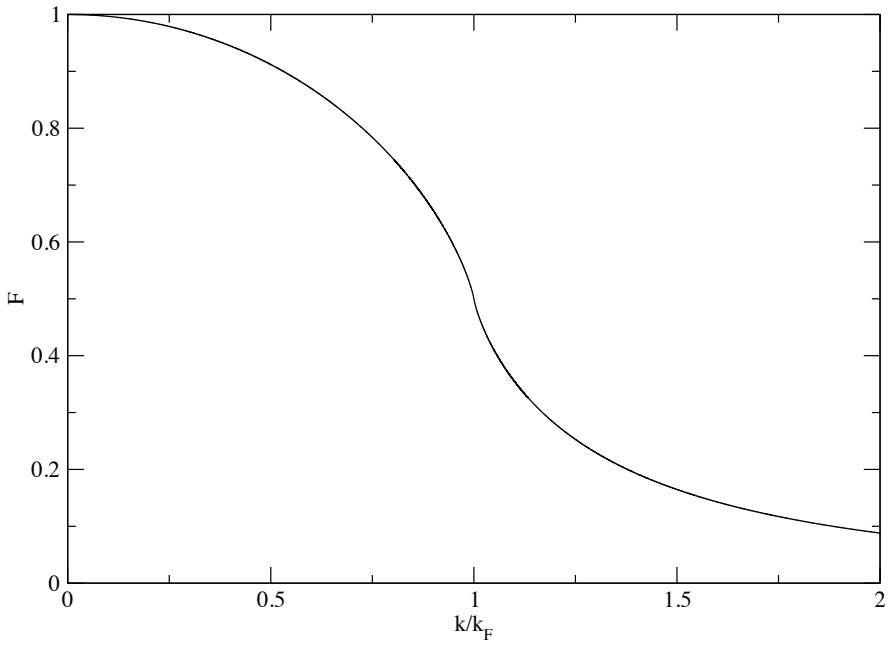
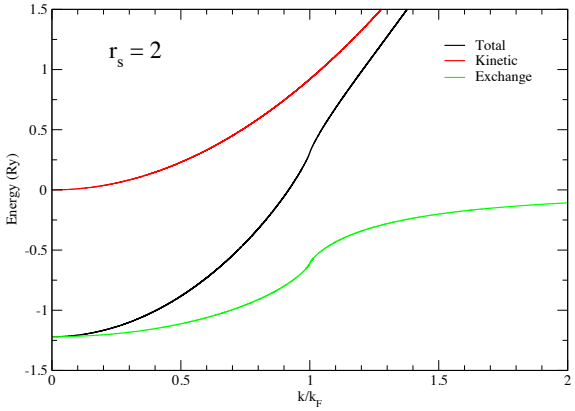
$$F(x)=1/2+(1-x^2)/(4x)\ln|(1+x)/(1-x)|$$



HF band energy



PHYSICAL REVIEW B **77**, 035131 (2008)

Many-body local fields theory of quasiparticle properties in a three-dimensional electron liquid

George E. Simion* and Gabriele F. Giuliani

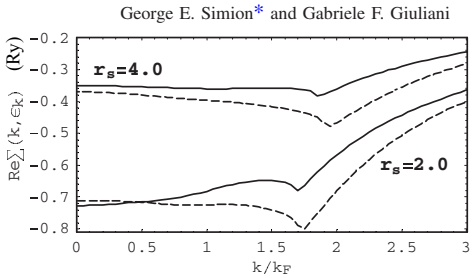


FIG. 5. Real part of the self-energy. Solid line: full theory; dashed line: RPA.

Self-consistent GW_0 results for the electron gas: Fixed screened potential W_0 within the random-phase approximation

Ulf von Barth and Bengt Holm

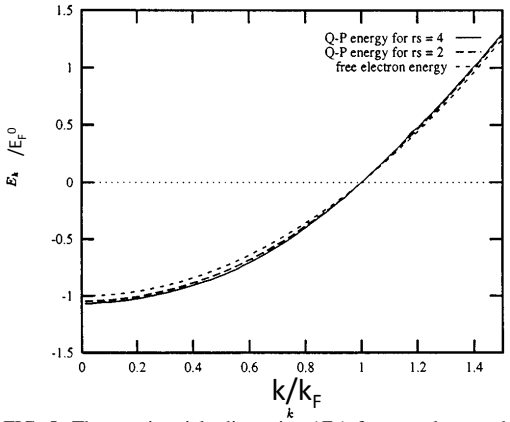


FIG. 5. The quasiparticle dispersion ($E_{\mathbf{k}}$) for two electron densities, $r_s=2$ and $r_s=4$ where r_s is the usual electron gas parameter. The largest change in the bandwidth occurs for $r_s=4$.

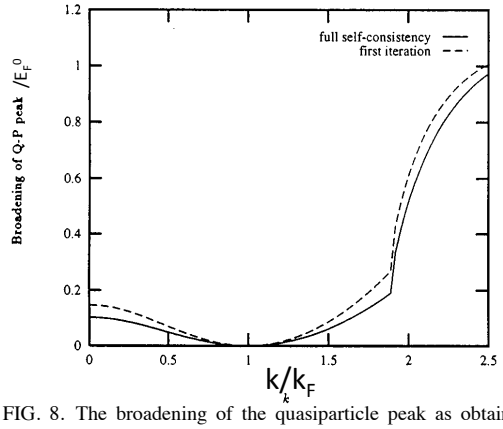
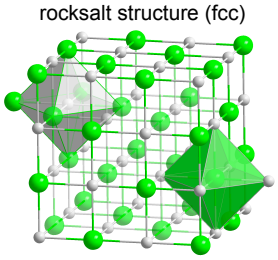


FIG. 8. The broadening of the quasiparticle peak as obtained from the spectral function (multiplied by π) of the self-energy evaluated at the quasiparticle energy. The sharpening of the quasiparticle peak due to self-consistency is evident ($r_s=4$).

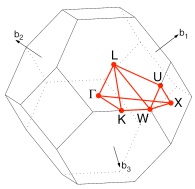
Band structure of NaCl in HF and GW vs experiment

$\varepsilon_\infty = 2.35$

rocksalt structure (fcc)



fcc Brillouin zone



FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

Chemical Physics Letters 285 (1998) 174–179

A Hartree–Fock ab initio band-structure calculation employing Wannier-type orbitals

Martin Albrecht [a], Alok Shukla [a], Michael Dolg [a], Peter Fulde [a], Hermann Stoll [b]

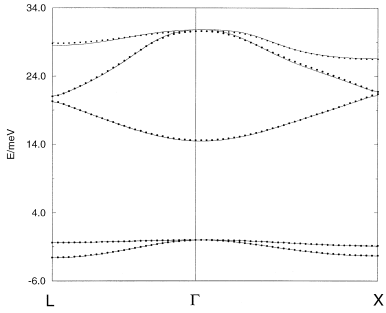


Fig. 1. Hartree–Fock band structure for NaCl. The highest three valence bands (the upper one being degenerate) as well as the lowest three conduction bands are displayed. The solid line shows results of the present work. For comparison, the results obtained by CRYSTAL95 are shown as dotted lines.

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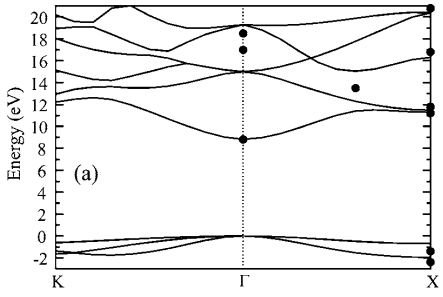
Quasiparticle bands and optical spectra of highly ionic crystals: AlN and NaCl

F. Bechstedt, K. Seino, P. H. Hahn, and W. G. Schmidt*



Quasiparticle bands for *rs*-NaCl. The filled circles indicate measured band positions