Acta Cryst. (1992). A48, 544-554

The Electronic Charge Distribution in Crystalline Silicon: Comparison of

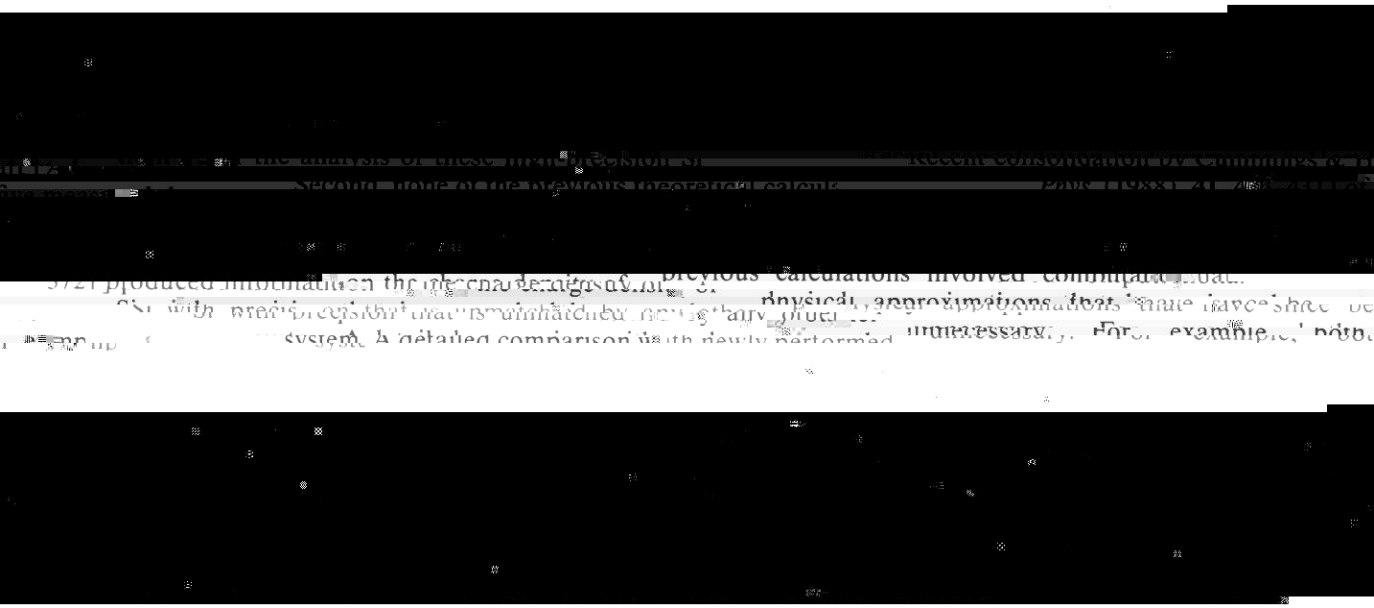

Table 1. *Dynamic (F) and static (ρ) structure factors for silicon*

The experimental data (corrected for anomalous dispersion and nuclear scattering), including the estimated standard deviations σ [illegible]

	10.6025		2.9	−3	10.455	−148	[illegible]	[illegible]
220	8.397	8.3881	2.2	−9	8.590	62	8.665	8.6553
311	7.694	7.6814	1.9	163	7.814	133	8.033	8.0204
222	0.181	0.1820	1.0	[illegible]	0.000	−182	0.168	0.1908
[illegible]	[illegible]	[illegible]	2.0	−14	5.502	−30	6.030	[illegible]
444	4.115	4.1239	1.8	−9	4.107	[illegible]	4.968	[illegible]
551	3.931	3.9349	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	2.331	[illegible]	2.5	2.6	11	1.542	10	2.331

[illegible] static structure factor [illegible] smearing function [illegible] the local density theory (Kohn & Sham, 1965) [illegible] as [illegible] convolution of the αth site static [illegible] follows. (i) Core and valence wavefunctions are [illegible] $\rho_\alpha(\mathbf{G})$ and the αth site dynamic [illegible] treated on equal footing, avoiding the pseudopotential approximation. (ii) An accurate electron-gas correlation functional [illegible]

$$F_{\mathrm{dyn}}(\mathbf{G}) = \sum_{\alpha}^{M} \rho_\alpha(\mathbf{G}) T_\alpha(\mathbf{G}) \exp(-i\mathbf{G}\cdot\boldsymbol{\tau}_\alpha) \quad (1)$$

[illegible] potential or charge density [illegible] where $\boldsymbol{\tau}_\alpha$ is the position vector of any of the M atoms [illegible] the basis set consists of a mix between [illegible] is invoked [illegible] obtained [illegible] the total distribution into a linear superposition from [illegible] Schrödinger equation of crystal-bound atoms. Simple [illegible] scattering objects located at sites $\boldsymbol{\tau}_\alpha$, and [illegible] (e.g. Slater or Gauss) orbitals are avoided. (v) The [illegible] term associated with a [illegible] We use an overkill set of convergence parameters [illegible] oned exactly at site α with a term that smears this [illegible] (size of basis set, sampling of the Brillouin zone etc.) [illegible] simply formed position over space (Dawson, 1969) [illegible] so that the results reflect the under[illegible]

[redacted]

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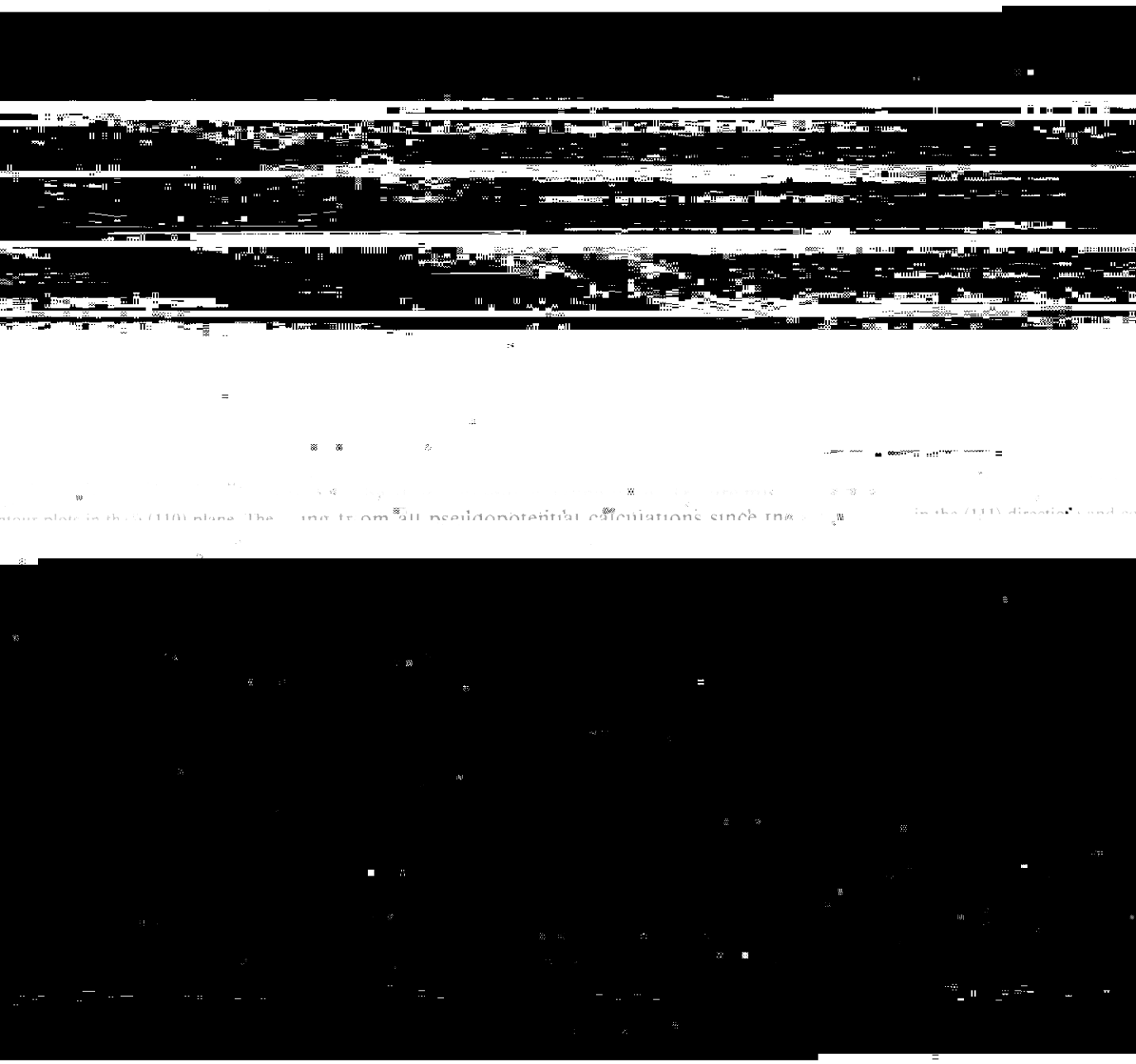
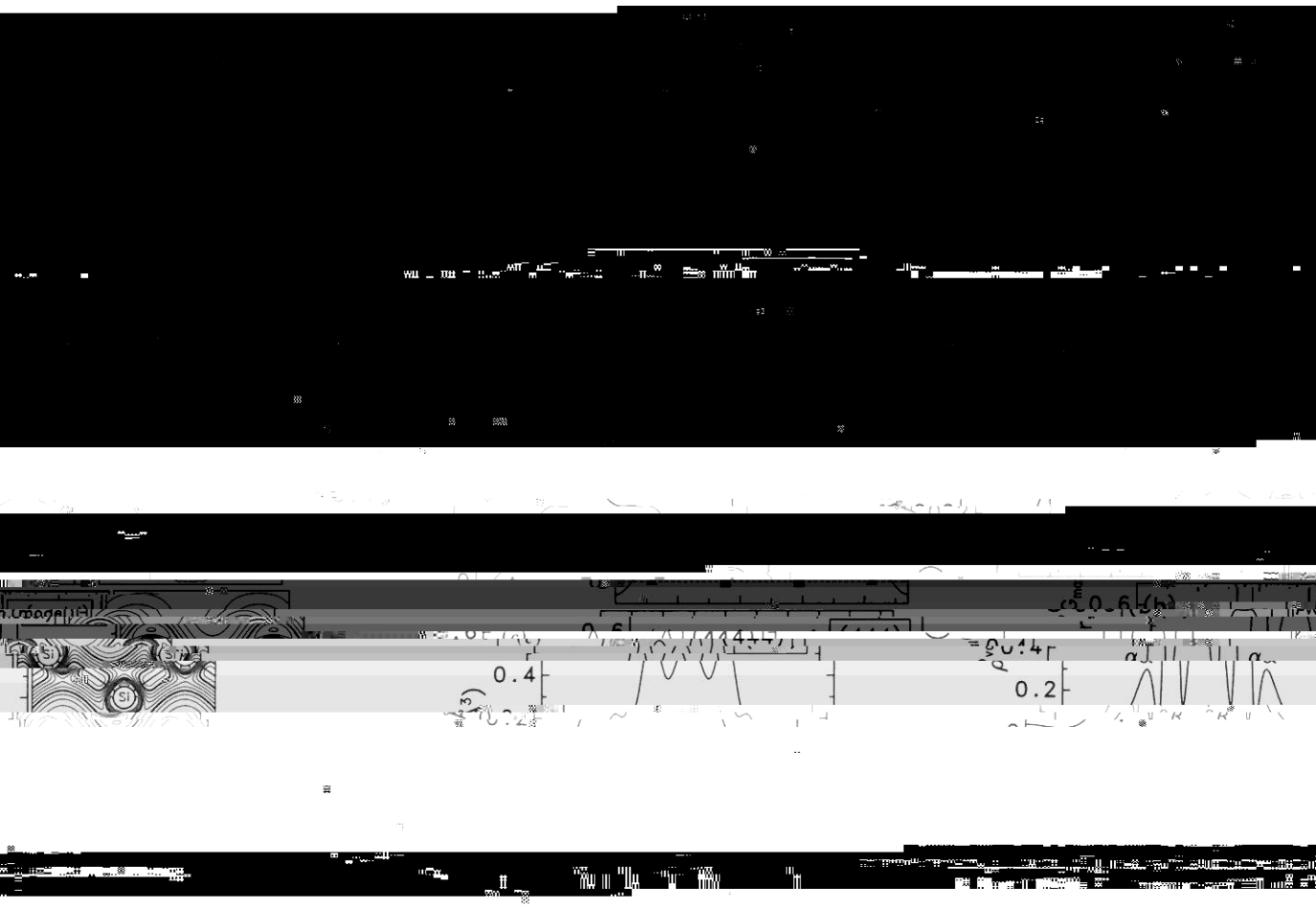
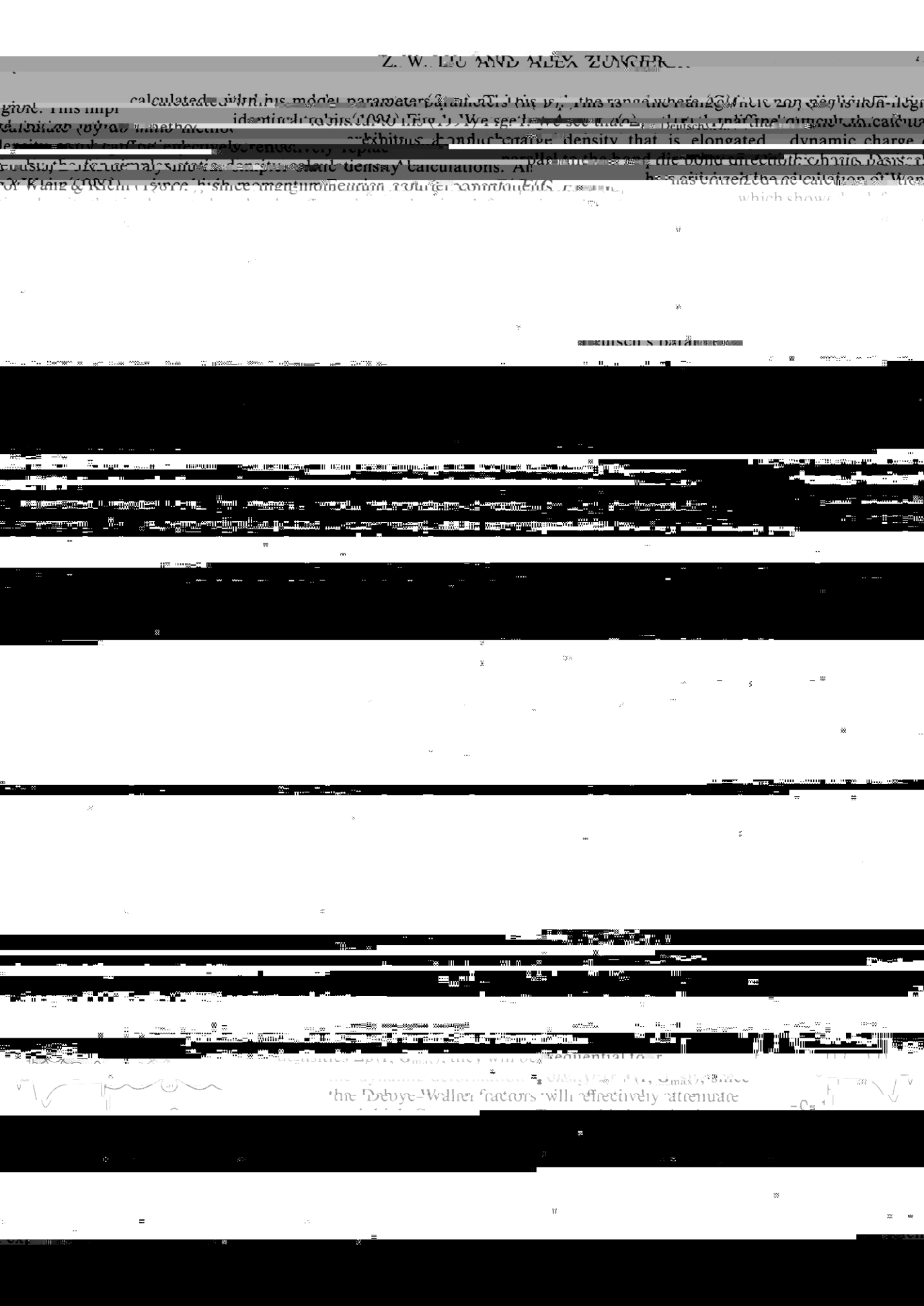


density. The inset denotes contour steps in e Å^{-3}


0.4
0.2



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WEYRICH, K. H. (1988). *Phys. Rev. B*, **37**, 10269.

cussions on the subject and to J. Spence and M. Hart for critical reading of the manuscript. This w