On the Calculation of Electric Field Gradients in Layered Compounds

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An analytical formula is derived for the electric field gradient (EFG) of a thin slab with an arbitrary charge density in the x-y-plane without z-dispersion, based on its Fourier expansion. It turns out that the EFG is dominated by the leading Fourier-coefficients for thin slabs and reduces to a contact-term proportional to the charge density at the nucleus in the truly two-dimensional case. An extension to charge density distributions which are factorizable into a function $f(x, y)$ and $g(z)$ is given with an example for a Gaussian $g(z)$. The consequences for EFGs in layered compounds such as TaS_2 and $TaSe_2$ are discussed.

Key words: Electric Field Gradients; Layered Compounds.