

EFGs on Surfaces – Experiment and Theory

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Experimental and calculated electric field gradients (EFG) on various probe atoms at different sites on metal surfaces, are reviewed. The calculations are based on the discrete variational method (DVM) molecular/cluster approach within the local density approximation and the experimental data are mostly obtained with the time differential perturbed angular correlation (TDPAC) method. Recent observations of an increasing EFG with temperature for adsorbed Se on (111) metal surfaces are explained as due to an outward probe relaxation, resulting in an increased EFG. This means that positive EFGs at (111) sites increase whereas negative EFGs at (001) surfaces reduce in magnitude. Previously unpublished results for various Cd-probe sites at Pd(110) are also discussed in detail.

Key words: Electric Field Gradient; Surface.