

A MAJOR UPDATE OF X'PERT HIGHSCORE PLUS

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In this presentation we will show some of the features of a new major release of our phase analysis software package X'Pert HighScore Plus. The demonstration will cover features like: Clustering of all candidates of a search-match run to get a fast overview hiding silly duplicates; a completely reprogrammed profile fitting engine, using a state of the art non-linear solver; seamlessly coupled Line Profile Analysis options; a strongly improved cluster analysis with speed gains of about a factor 5, covering new options for better handling of non-XRPD data as well as display of semi-transparent cluster spheres; seamless integration of charge flipping software with real-time update of calculated electron densities.

