Fast data sorting to distinguish unique single molecular break junction trajectories

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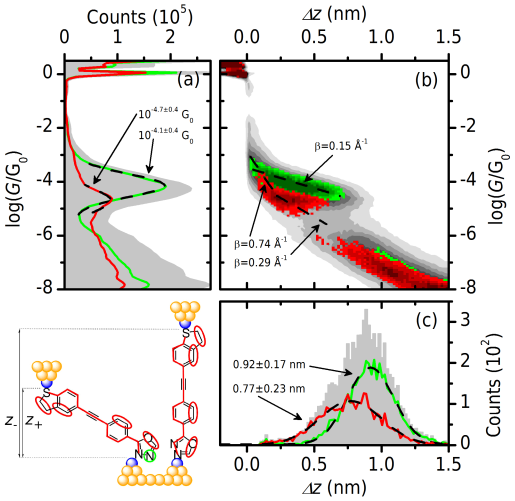
A simple and fast analysis method to sort large data sets into groups with shared distinguishing characteristics is described, and applied to single molecular break junction data. The method successfully sorts data sets without the need to assert any specific hypothesis about the expected features within the data. The method is applied to mixtures of two molecules with identical anchor groups, similar lengths, but either a π (high conductance) or σ (low conductance) bridge. The mixed data is sorted into break junctions containing one molecule or the other. The method also distinguishes between two junction geometries in measurements of the π bridged molecule alone[1].



[1] J.M. Hamill, X.T. Zhao, G. Mészáros, M.R. Bryce, and M. Arenz **(2017)**. "Fast data sorting with modified principal component analysis to distinguish unique single molecular break junction trajectories." arXiv:1705.06161 [cond-mat.mes-hall]