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Novel Application of Cluster Analysis to Transport Data in Single Molecule Break Junctions BEN WU[1], JEFFREY IVIE[2], TYLER JOHNSON[3], ROLAND HIMMELHUBER[4], OLIVER MONTI[5], Univ of Arizona —
Single molecule based devices represent the ultimate limit in device design, but uncovering the major factors that determine energy level alignment in single molecule junctions and their effect on the charge transport properties of single molecules is still a major challenge. Analysis of break junction data using a novel density based hierarchical clustering algorithm reveals the deep structure of the highly stochastic data that will help hypothesis-driven elucidation of some of the key parameters for quantum transport. The strength of this approach is its scale-invariance and the identification of nested structure that may be overlooked by standard data analysis techniques. The statistical relevance of identified clusters can be gauged using a density based validation index.

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