Kernel principal covariates regression

These datasets contain low-dimensional representations of the structures, or the atom-centered environments within them, using a dimensionality reduction algorithm called KPCovR (Kernel Principal Covariates Regression), that aims at obtaining a low-dimensional representation that reproduces a large fraction of the intrinsic structural variability of the structures, and correlates linearly with the properties associated with them. The emphasis that is given to the variance maximization or the property regression task is controlled by a parameter α, with $\alpha=0$ indicating complete focus on regression, and $\alpha=1$ being equivalent to principal component analysis.

Maps are visualized using chemiscope, an interactive structure/property explorer for materials and molecules.