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Local Crystallography
Analyzing atomic environments with statistical methods

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AI for atoms: How to machine learn STEM
December 10th, 2020

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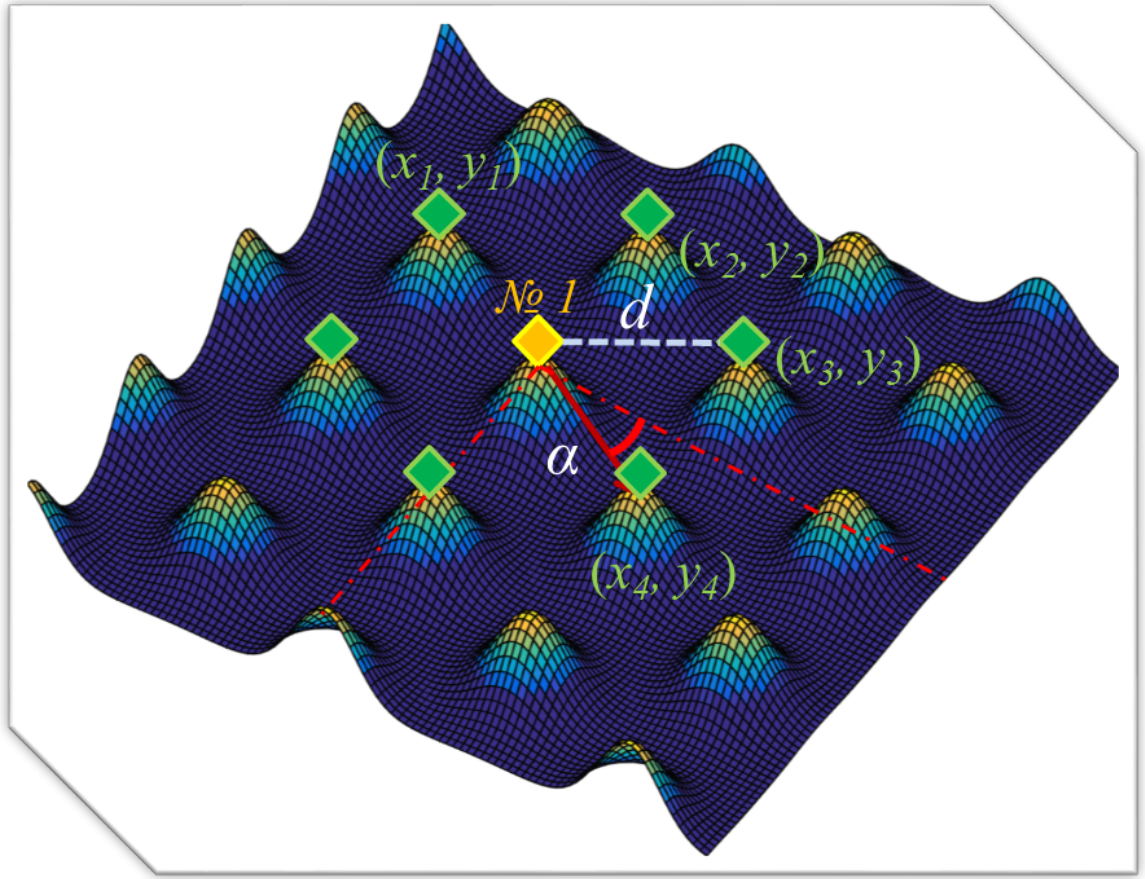
Atomic positions: Obtaining statistics



- Find atoms using some algorithms
- Determine the distance from each individual atom to the *J* nearest neighbors, and compute the angles
- Iterate over all *N* atoms in image to build the matrix of size *N* x *J* x 2
- Compute statistics of this matrix. E.g., perform k-means or principal component analysis

Essential: PCA and K-means Clustering

Principal Component Analysis: Decomposition based on variance

$$A_i(U_j) = a_{ik} w_k(U_j)$$ ← 'Principal Components'

$$a_{ik} \equiv a_k(x, y)$$ ← 'Loadings'

- Components are orthogonal, loadings in order of maximum to minimum variance

K-means Clustering algorithm, to separate data ($x_1, x_2, \ldots, x_n$) into *k* clusters

$$\arg\min_{\boldsymbol{S}} \sum_{i=1}^{k} \sum_{\mathbf{x} \in S_i} ||\mathbf{x} - \boldsymbol{\mu}_i||^2$$ where μ_i is the mean of points in S_i

(Determine **S** = $\{S_1, S_2, \ldots S_k\}$, such that within cluster sum of squares is minimized)

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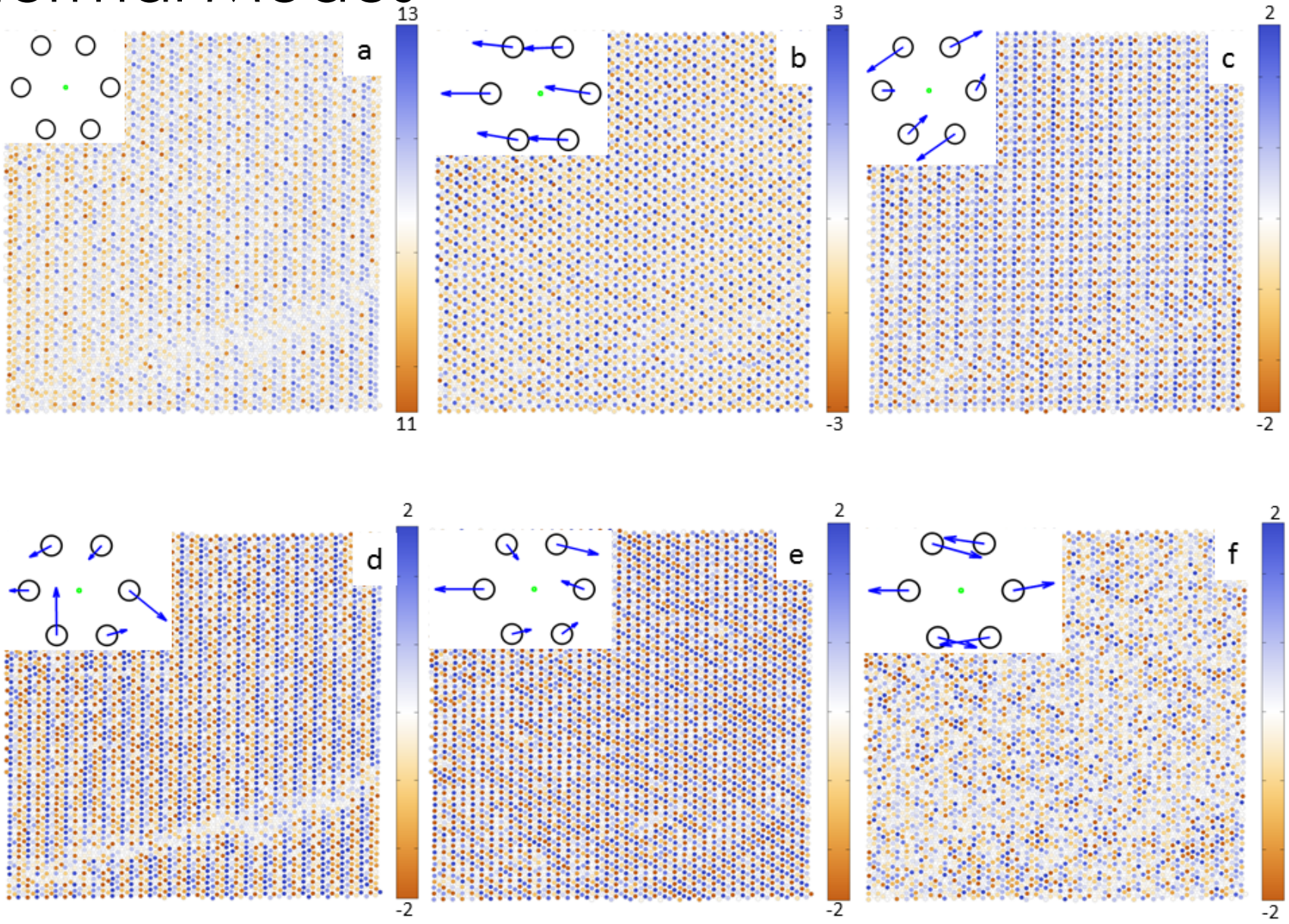
‘Normal Modes’



A. Belianinov *et. al.* Nature Communications, doi: 10.1038/ncomms8801 (2015)

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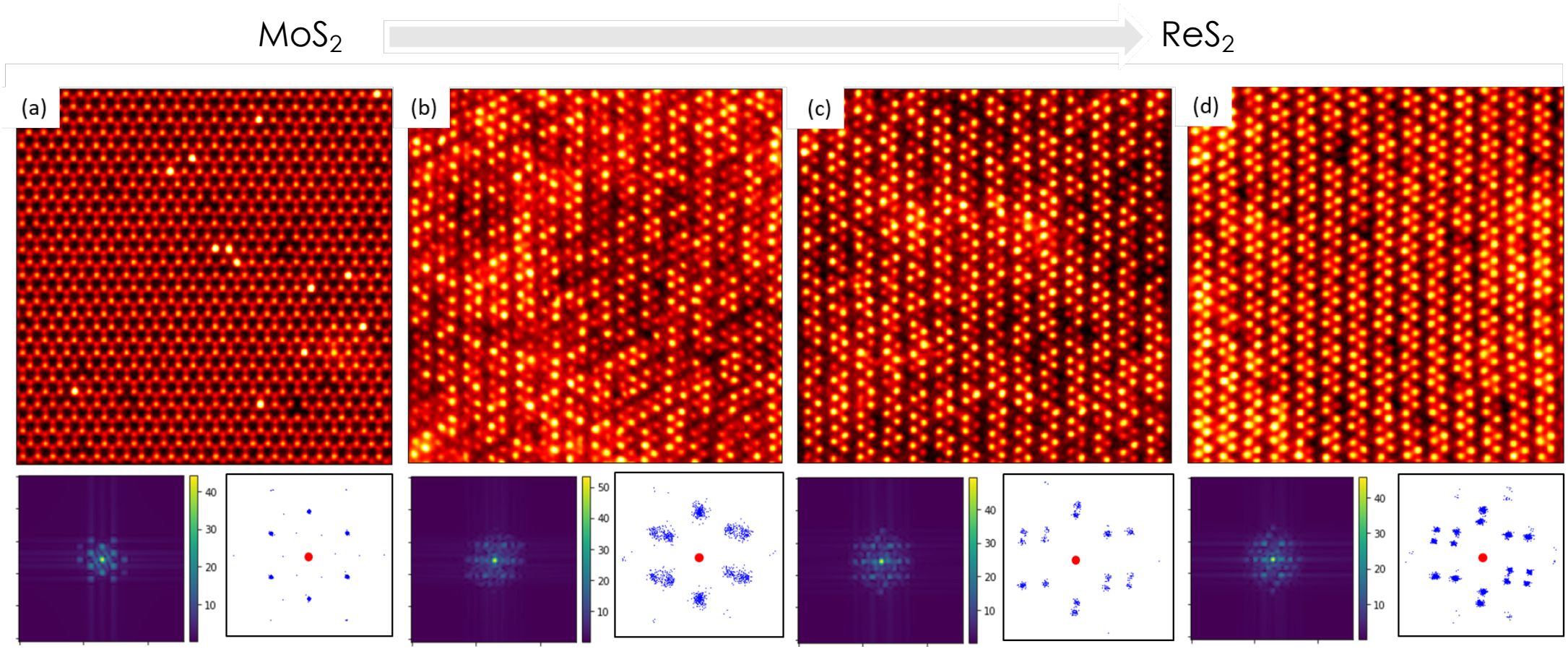
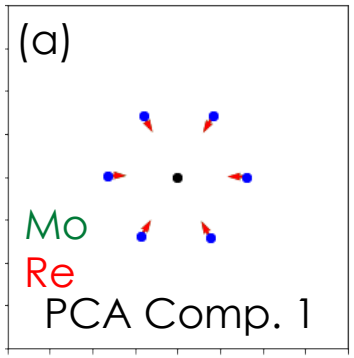
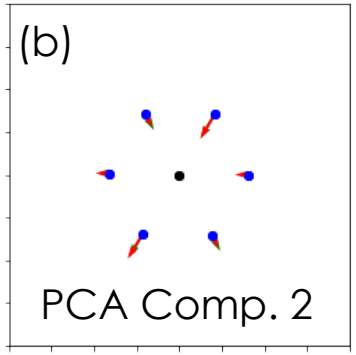
Can be used for understanding phase transitions

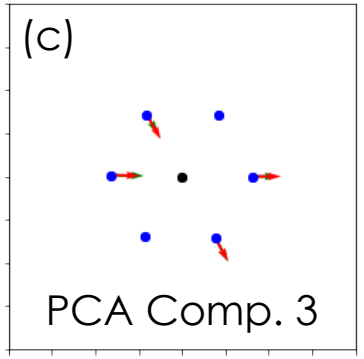


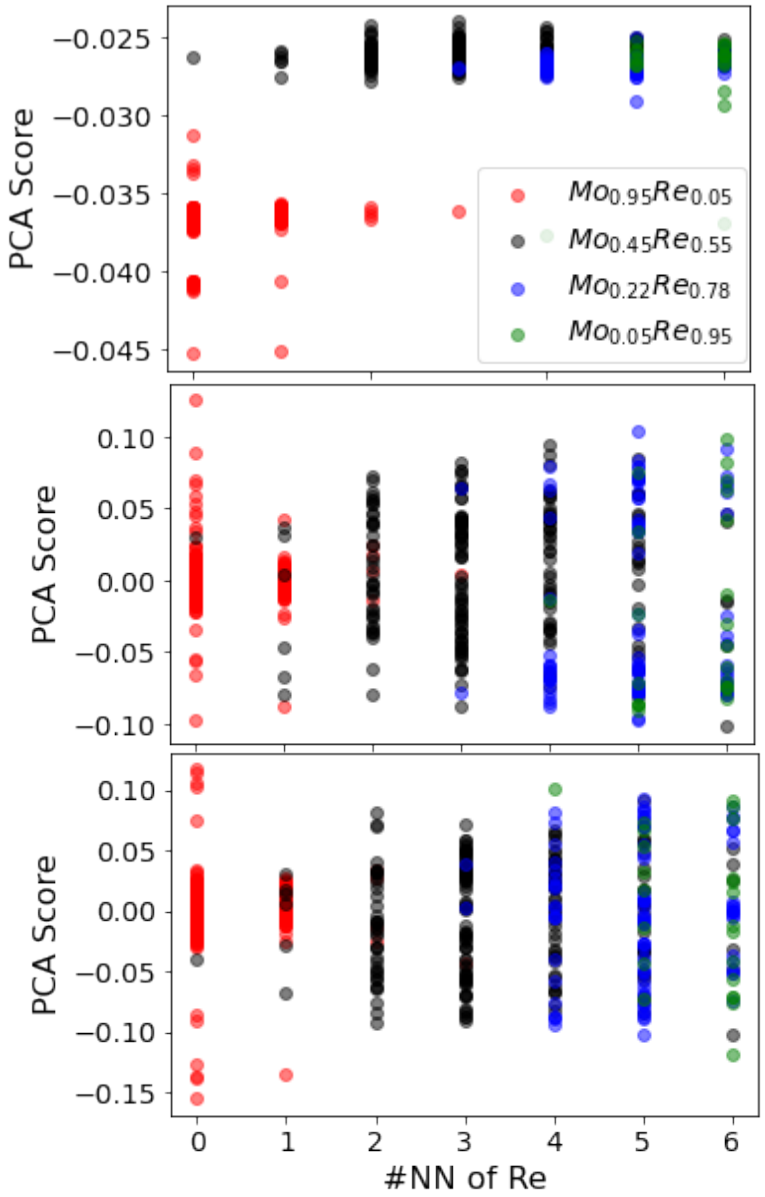
R. Vasudevan *et. al.* arXiv:2006.10001(2020).

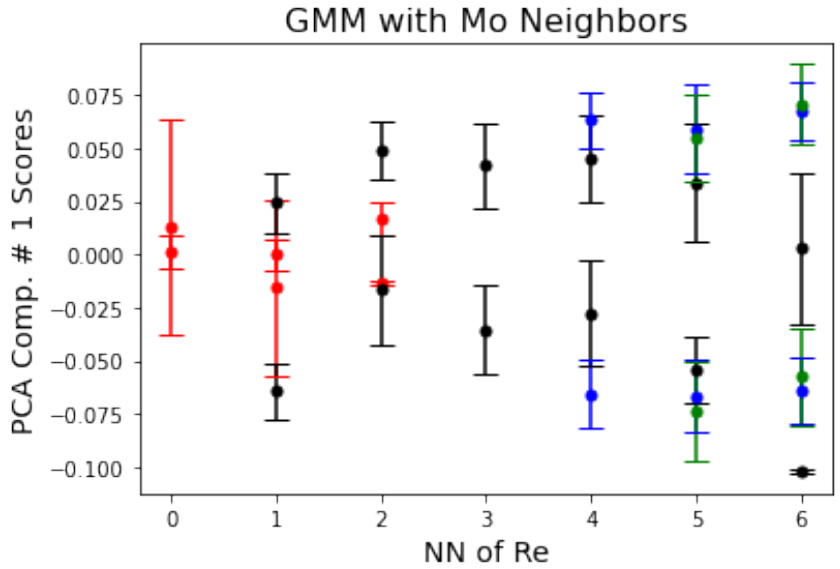
Can be used for understanding phase transitions











Overlap of the colors indicates that local chemistry is driving phase transition