Prediction of nucleation in LJ systems

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Outline

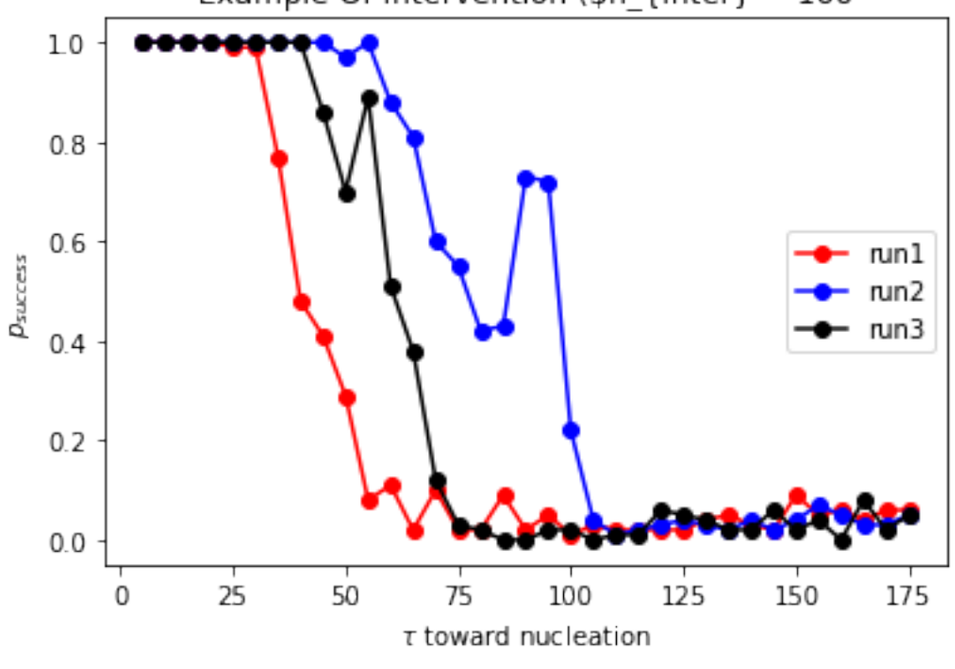
- Nucleation in Lennard Jones Dense Liquid
- SteinHardt Order Parameter and cluster analyses
- Machine Learning Prediction of nucleation probability

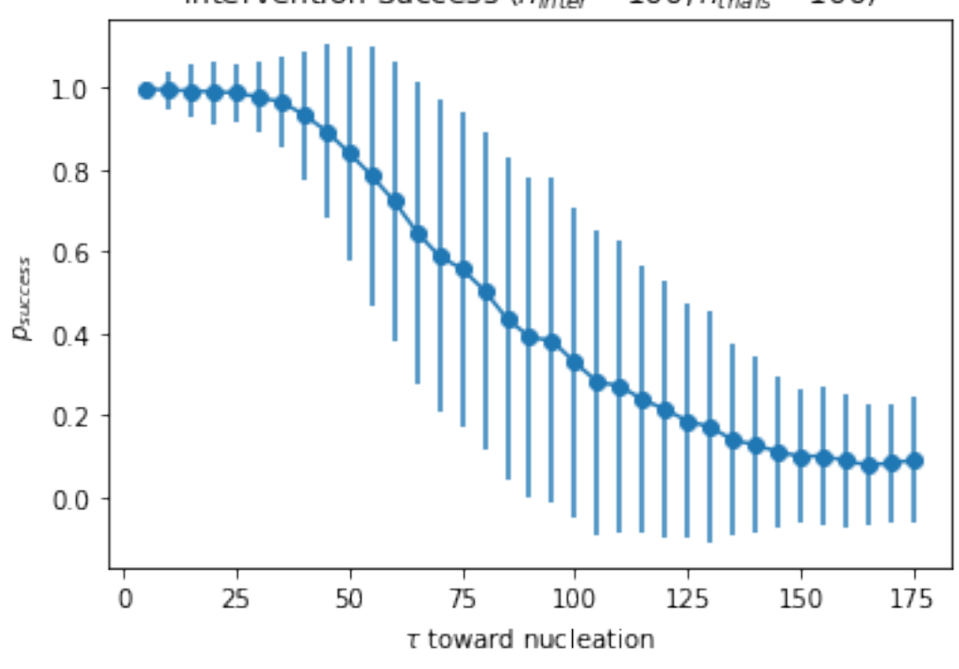
Nucleation Probability (Intervention)

Simulation Parameters

$$T = 0.55,\ N_{atom} = 4000,\ \rho = 0.95$$

Nucleation Criteria: Running Average of Temperature > 0.61 in a window of 10τ





Evolution of particles during Nucleation

During nucleation, some particles form lattices and become more and more “solid like”. there are three sets of parameters to describe spatial properties of a particle

- SteinHardt Order Parameter

$$q_l(i) = \sqrt{\frac{4\pi}{2l+1}\sum_{m=-l}^{l}|q_{lm}(i)|^2}$$

$$q_{lm}(i) = \frac{1}{N(i)}\sum_{j=1}^{N(i)} Y_{lm}(\hat{\mathbf{r}}_{ij})$$

- Average Bond Parameter (Wolfgang Lechner 2008)

$$\langle q_l\rangle(i) = \sqrt{\frac{4\pi}{2l+1}\sum_{m=-l}^{l}|\bar{q}_{lm}(i)|^2}$$

$$\bar{q}_{lm}(i) = \frac{1}{\tilde{N}(i)}\sum_{j=1}^{\tilde{N}(i)} q_{lm}(j).$$

- Local Order Parameter

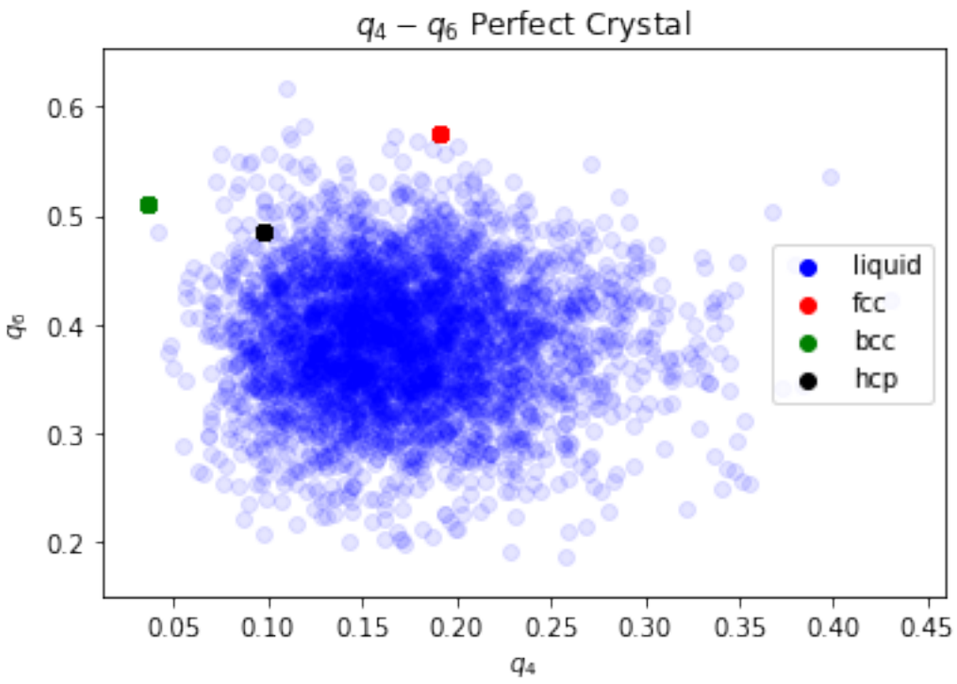
$$q_l^G(i) = \frac{1}{N(i)}\sum_{j=1}^{N(i)}\frac{\sum_{m=-l}^{l} q_{lm}(i)q_{lm}^*(j)}{\sqrt{\sum_{m=-l}^{l} q_{lm}(i)q_{lm}^*(i)}\sqrt{\sum_{m=-l}^{l} q_{lm}(j)q_{lm}^*(j)}}$$

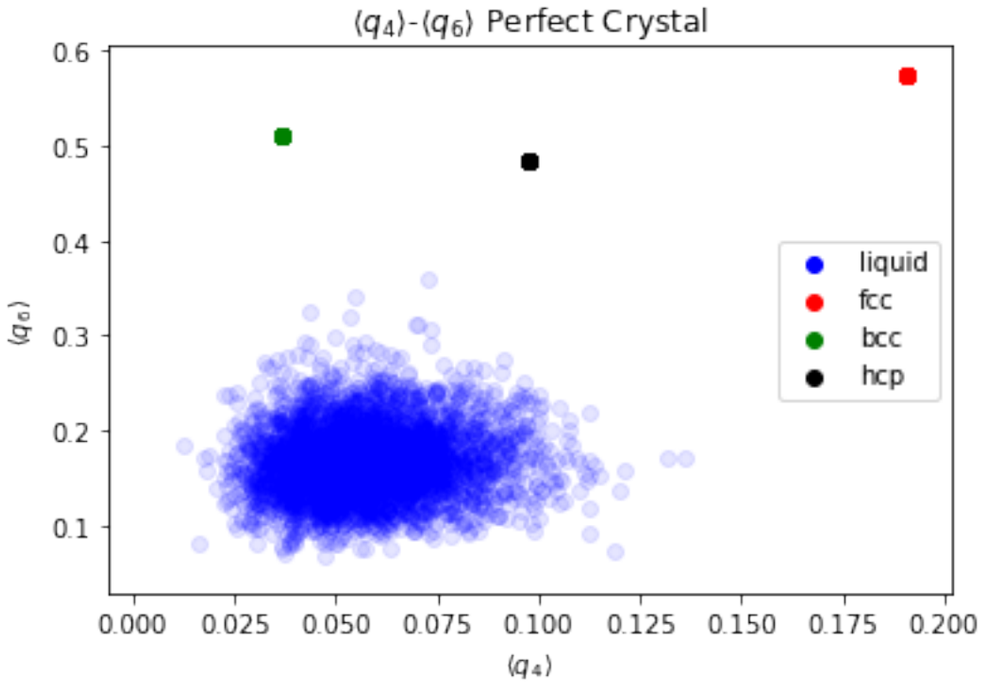
Example: Solid-Like Particles

$q_4 - q_6$

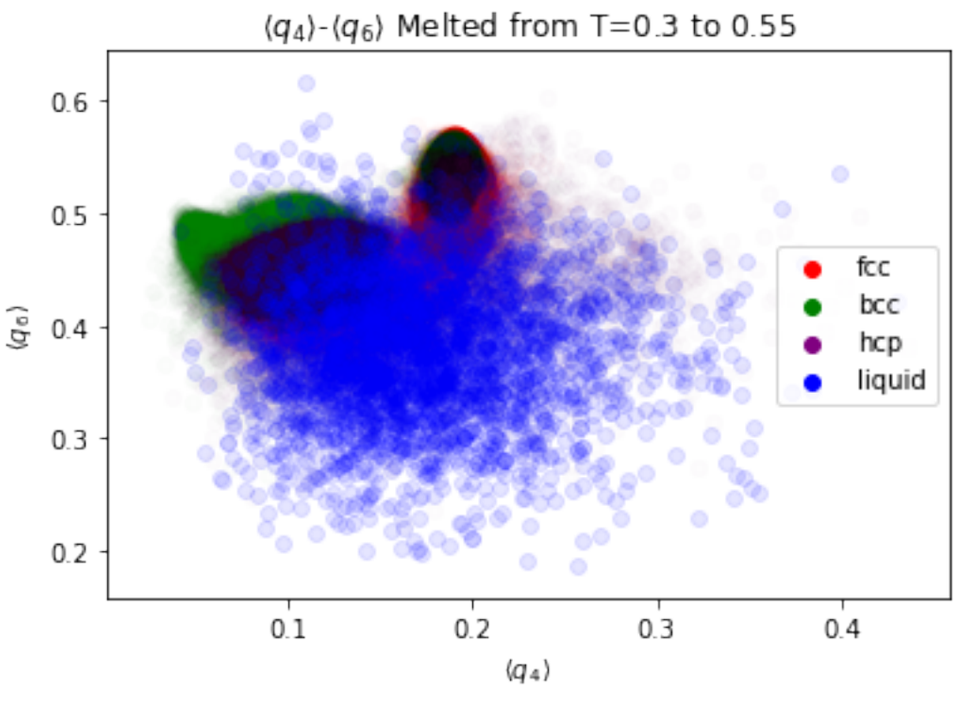
$\langle q_4 \rangle - \langle q_6 \rangle$

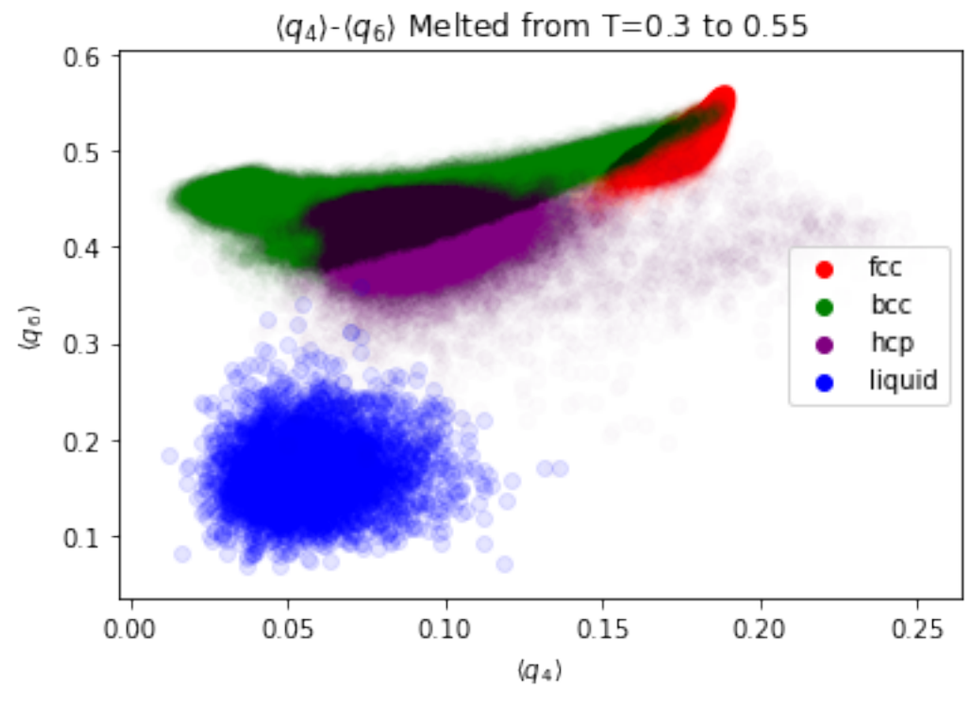
Perfect Crystal





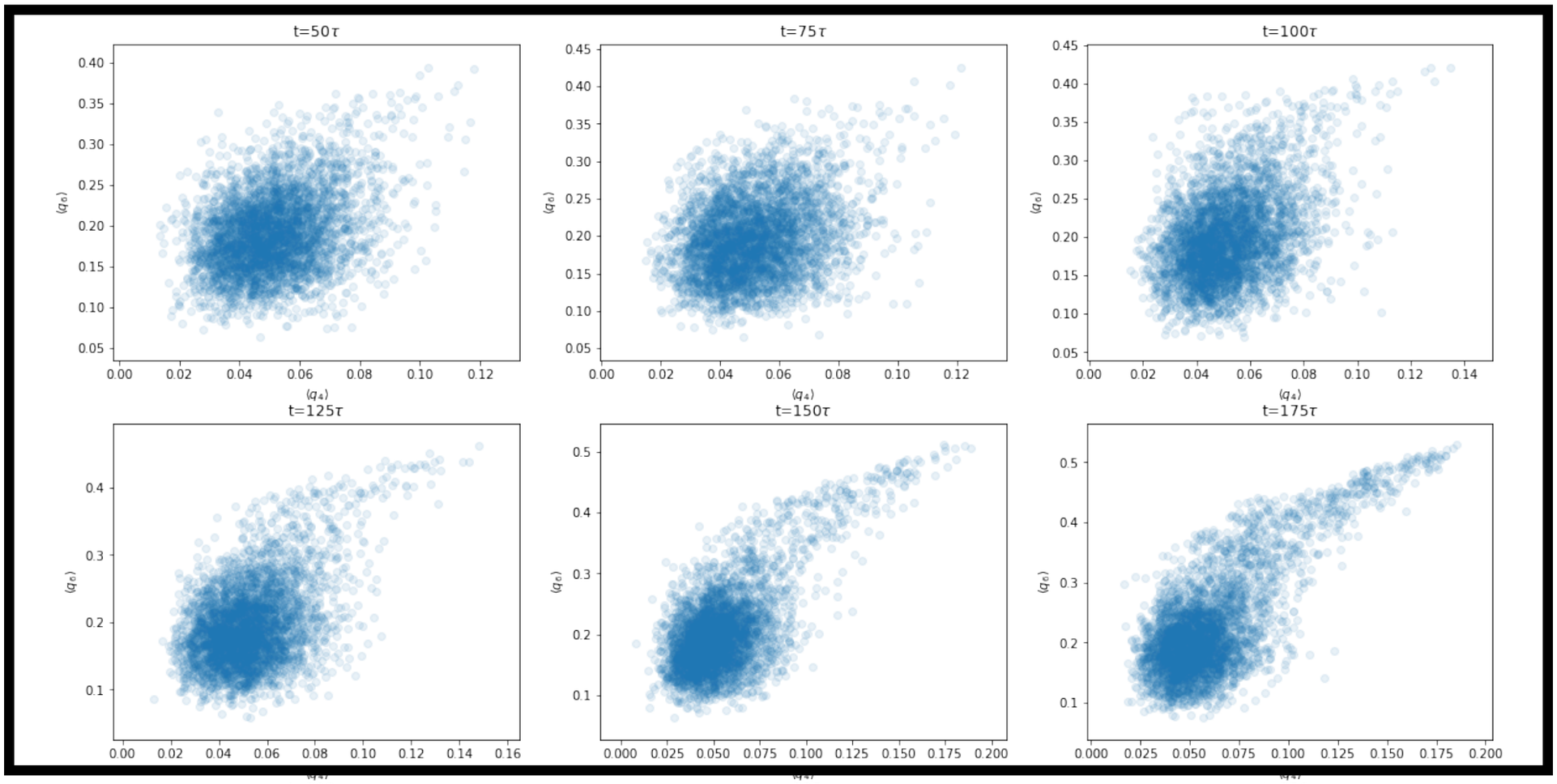
Melted Trajectory





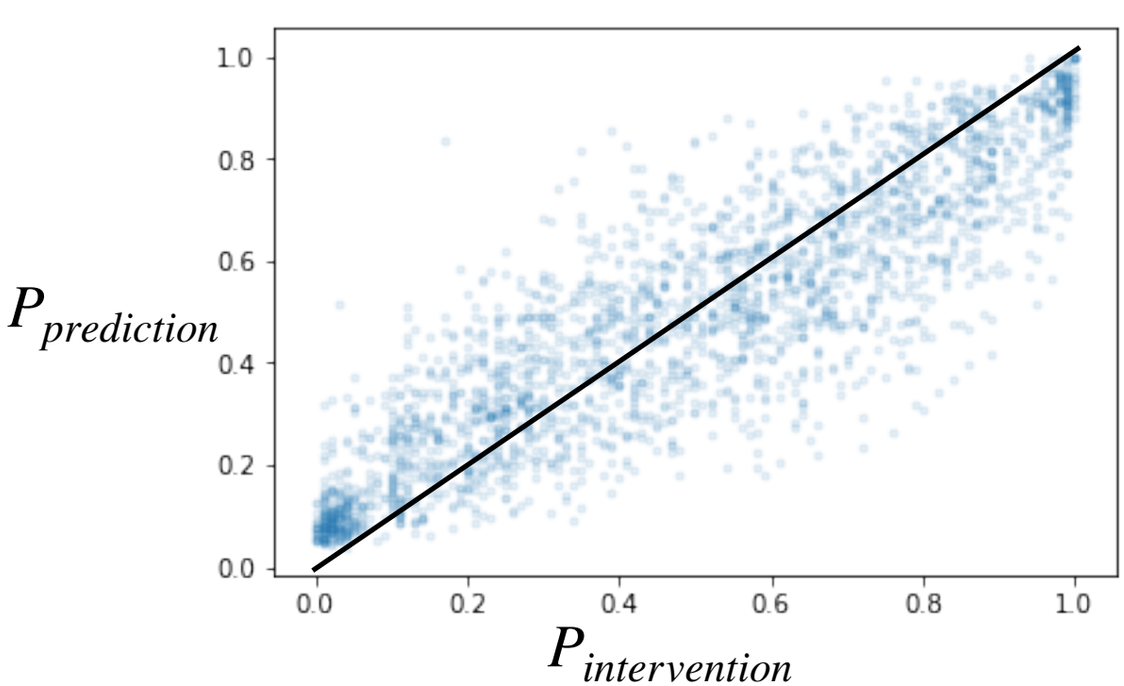
Example: Trajectory of OP during nucleation

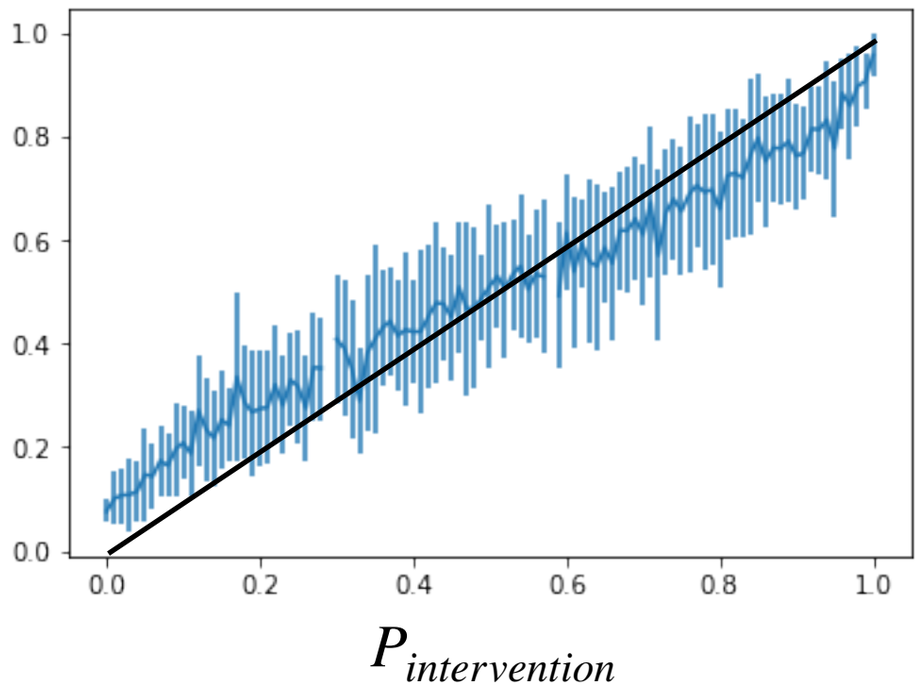
$\langle q_4 \rangle - \langle q_6 \rangle$



Most samples falls in the region

Deep learning prediction of Nucleation Probability



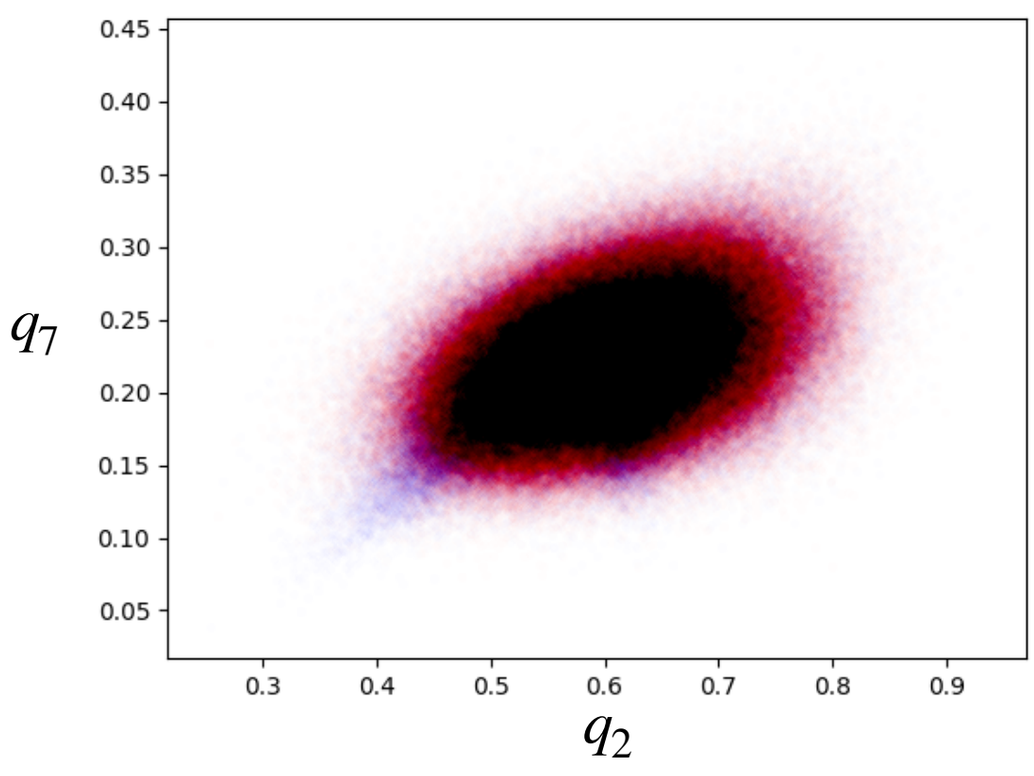


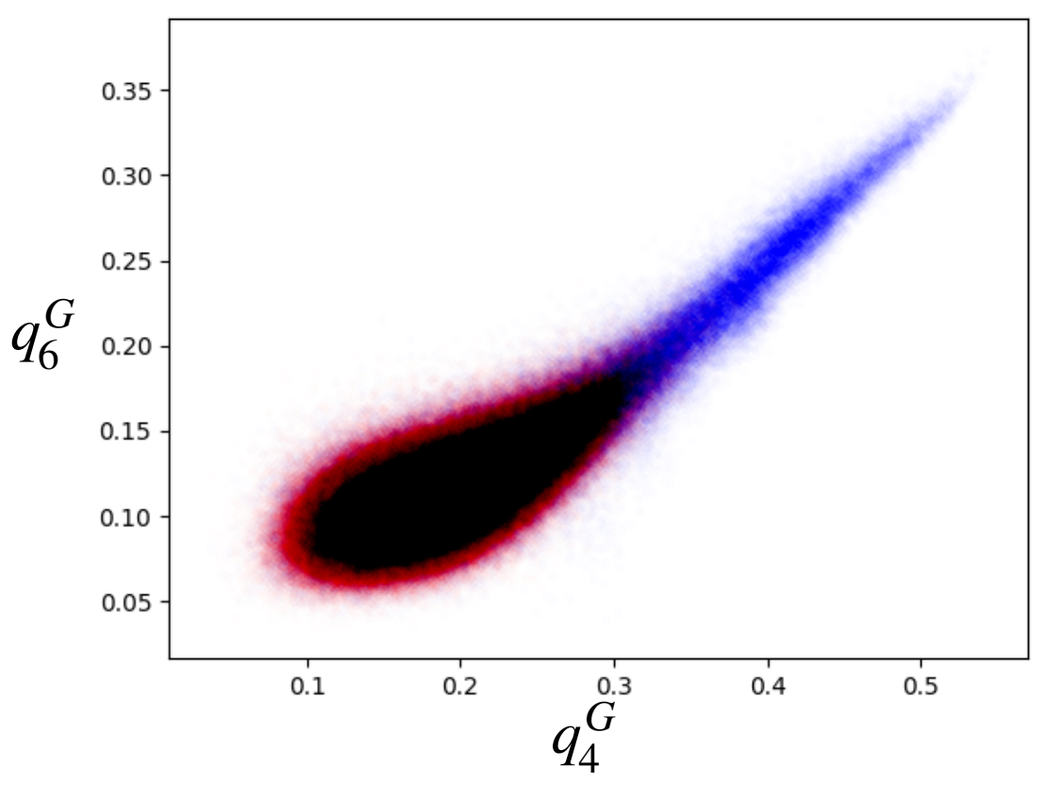
$$\langle q_4 \rangle - \langle q_6 \rangle$$

Which OPs are more relevant?

30 Order parameters:

$$q_3,\ q_4, \ldots,\ q_{12}$$
$$\langle q_3 \rangle,\ \langle q_4 \rangle,\ \ldots,\ \langle q_{12} \rangle$$
$$q_3^G,\ q_4^G,\ \ldots,\ q_{12}^G$$

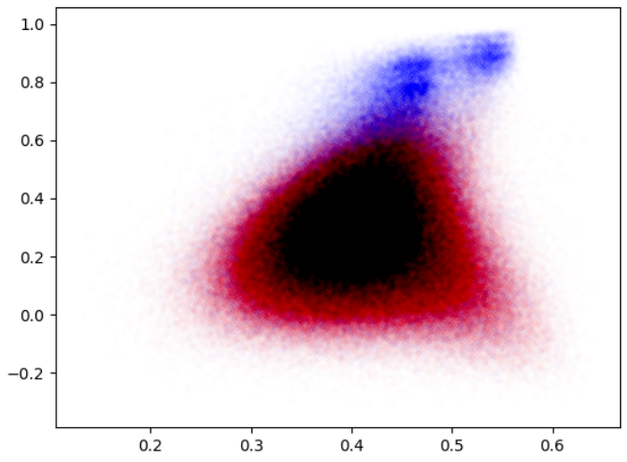




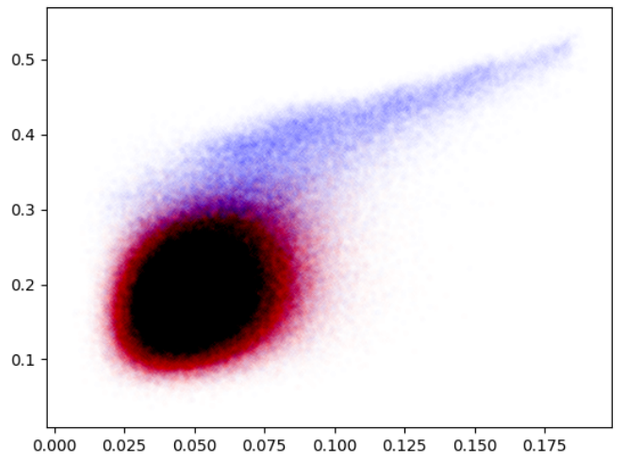
Which OPs are more relevant?

More Examples…

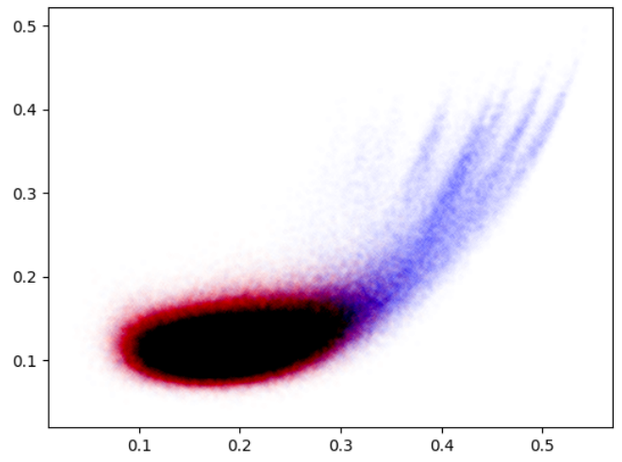
$q_6 - q_6^G$



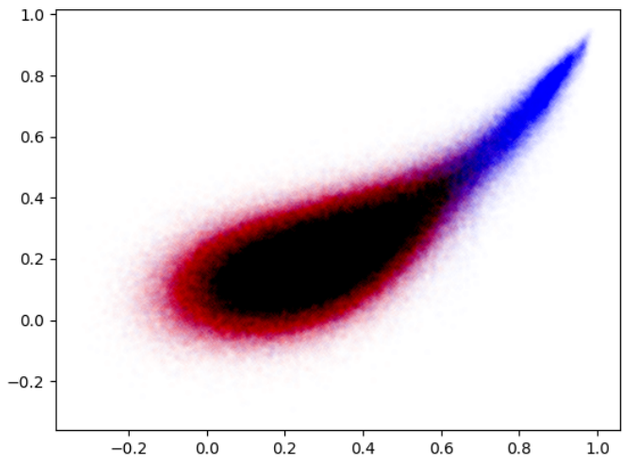
$\langle q_4 \rangle - \langle q_6 \rangle$



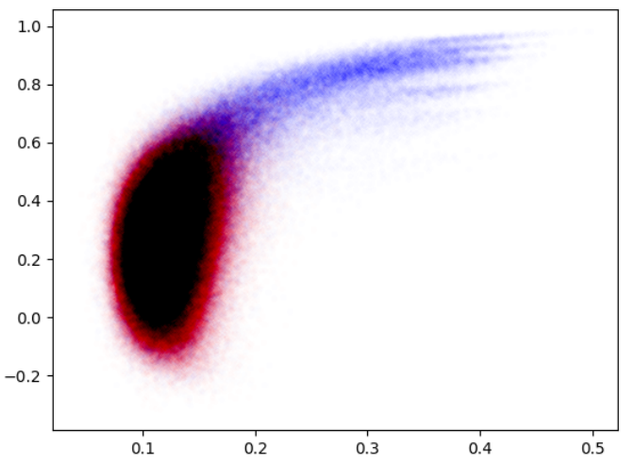
$\langle q_6 \rangle - \langle q_{12} \rangle$



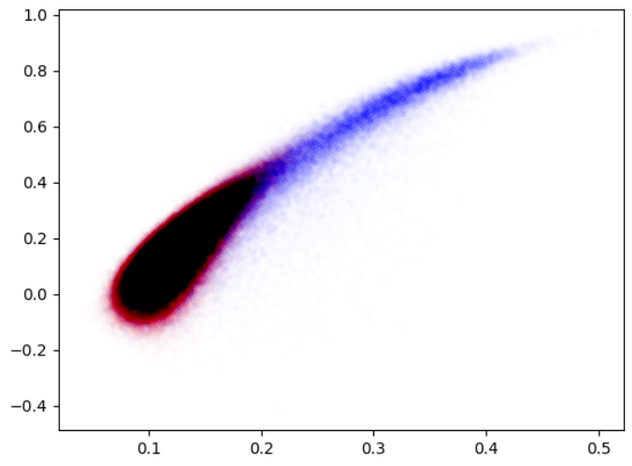
$q_4^G - q_6^G$



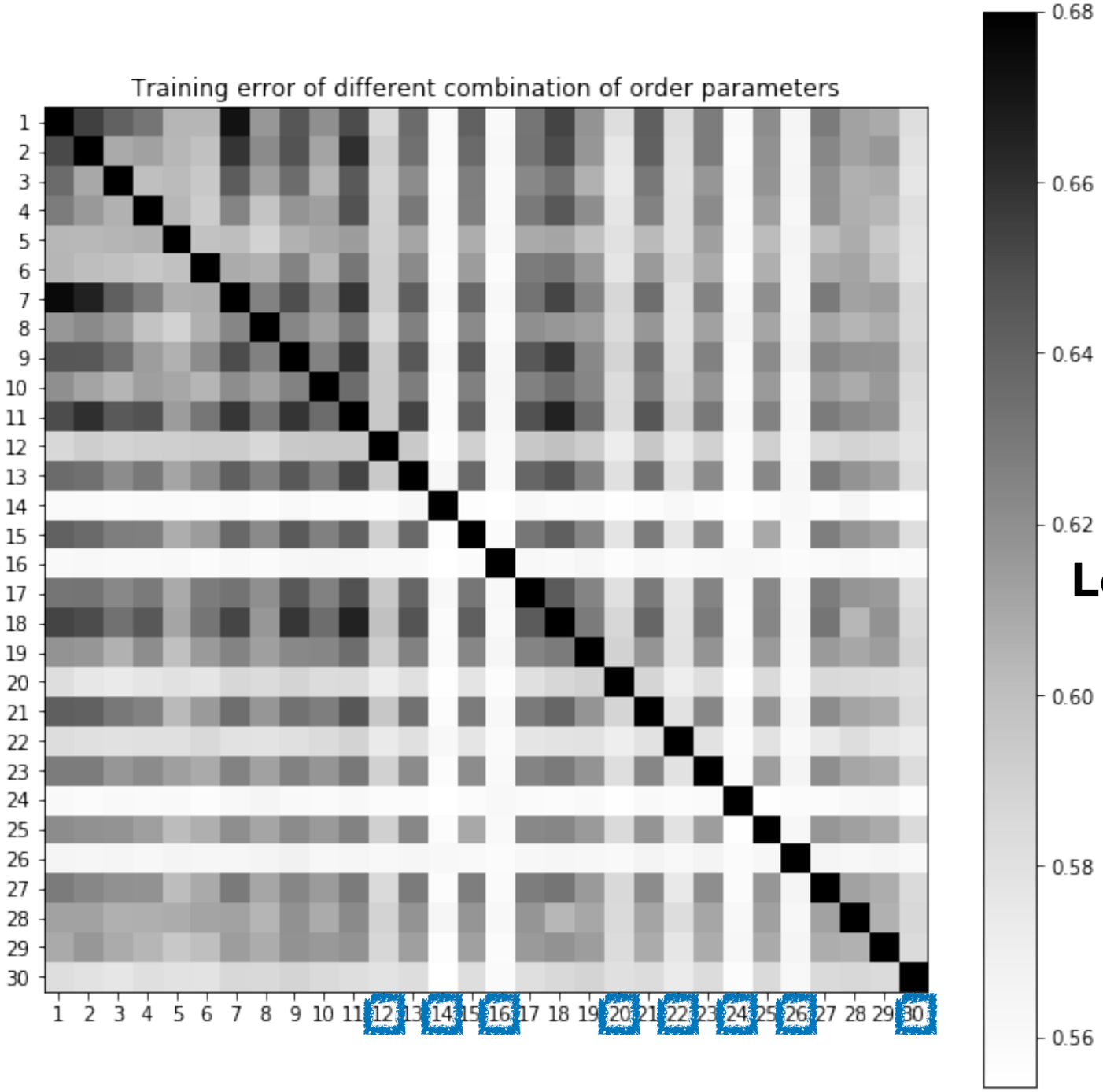
$\langle q_{12} \rangle - q_6^G$



$\langle q_{12} \rangle - q_{12}^G$



Which OPs are more relevant?



We use different combinations of order params to train the machine and measure the predicting power of each machine.
If a certain set of order parameter gives more accurate prediction, that means those parameters gives more information about nucleation

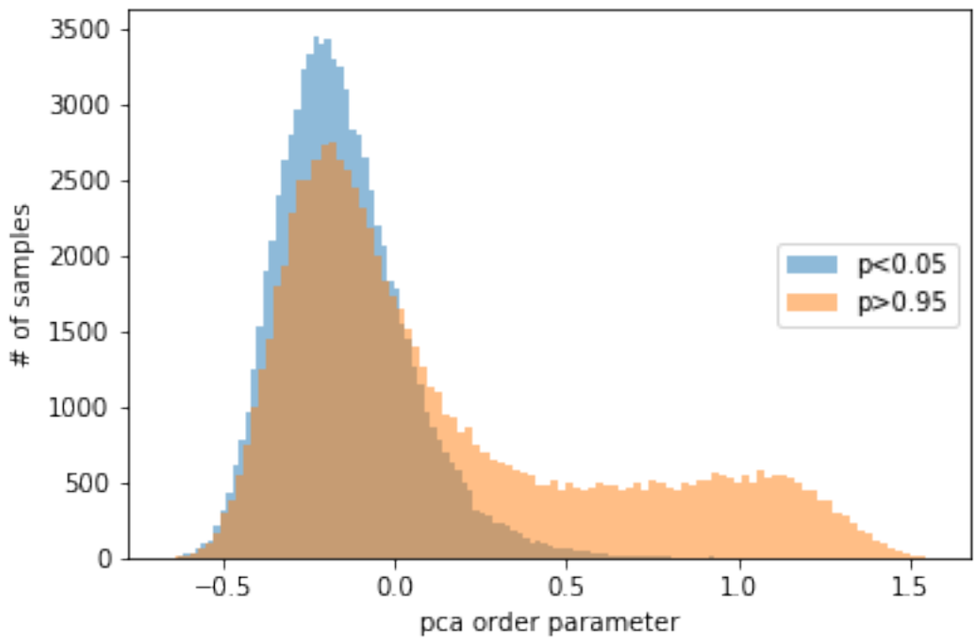
Important Order Params:

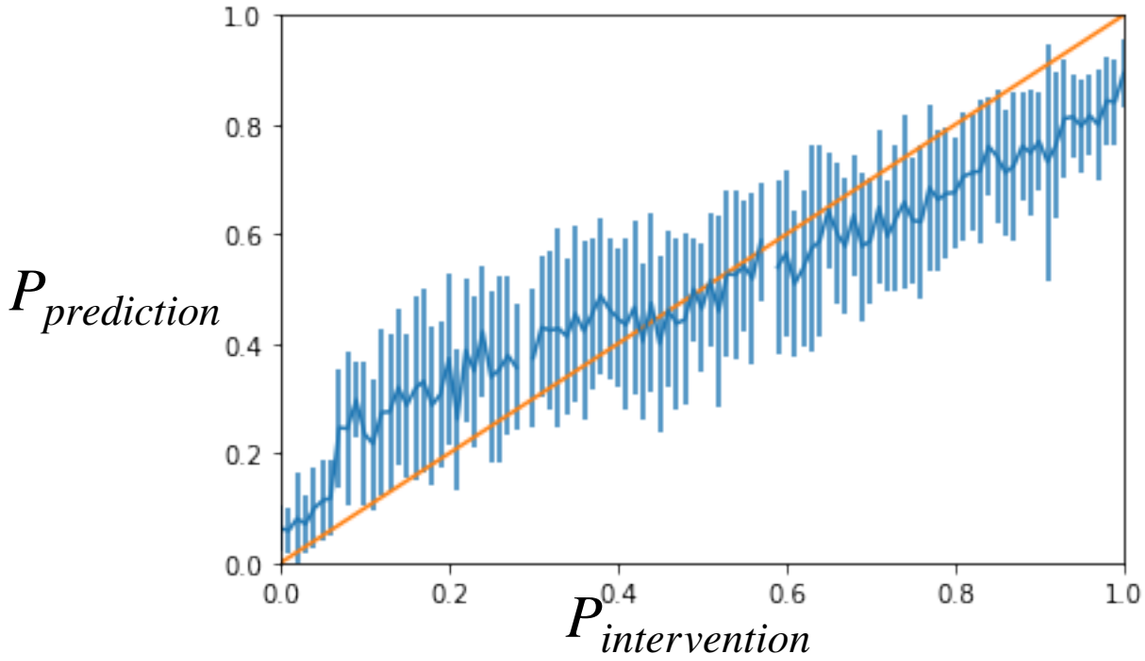
$$\langle q_4 \rangle,\ \langle q_6 \rangle,\ \langle q_8 \rangle,\ \langle q_{12} \rangle$$

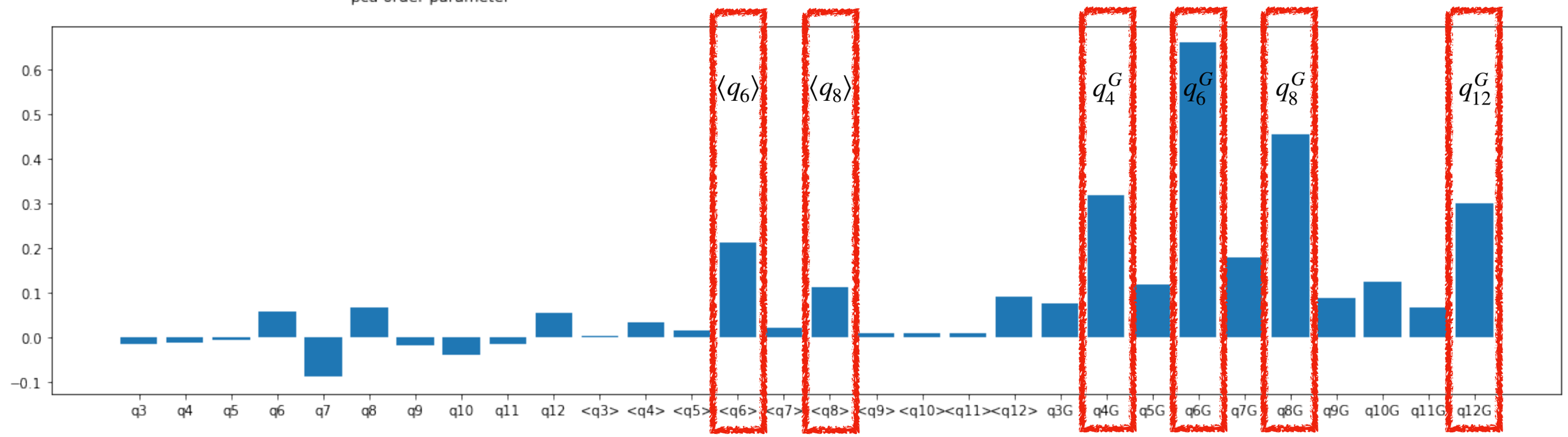
$$q_4^G,\ q_6^G,\ q_8^G,\ q_{12}^G$$

How about we use PCA?

Use only First PCA component







Conclusion

- 1. Using selected order parameters one can make predictions on nucleation in LJ simulation

- 2. By selecting different pairs of parameters in training, one can identify OPs that are more important in determining state of the nucleating system

- 3. PCA identifies most expressive order parameters, the result agrees with previous studies.