

Supplementary information

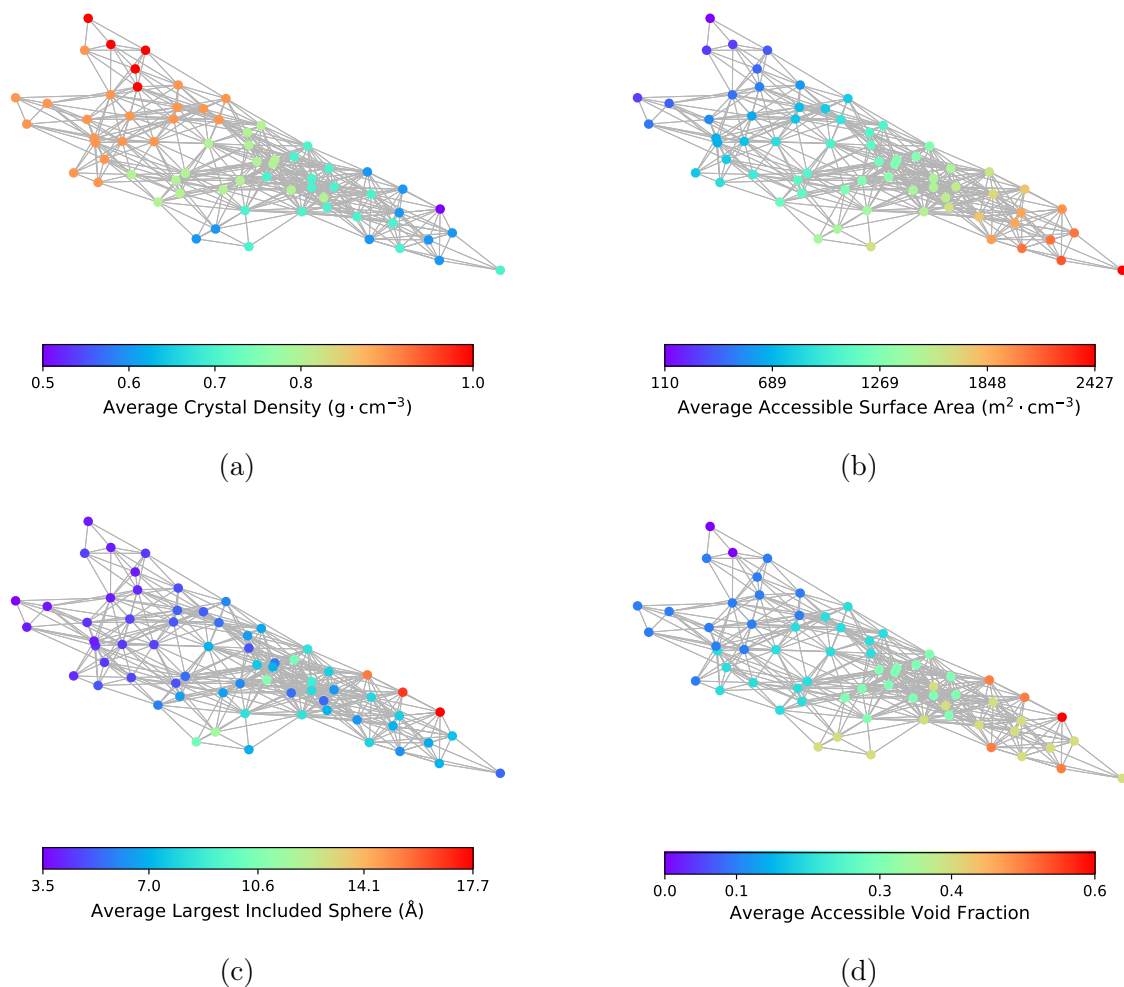
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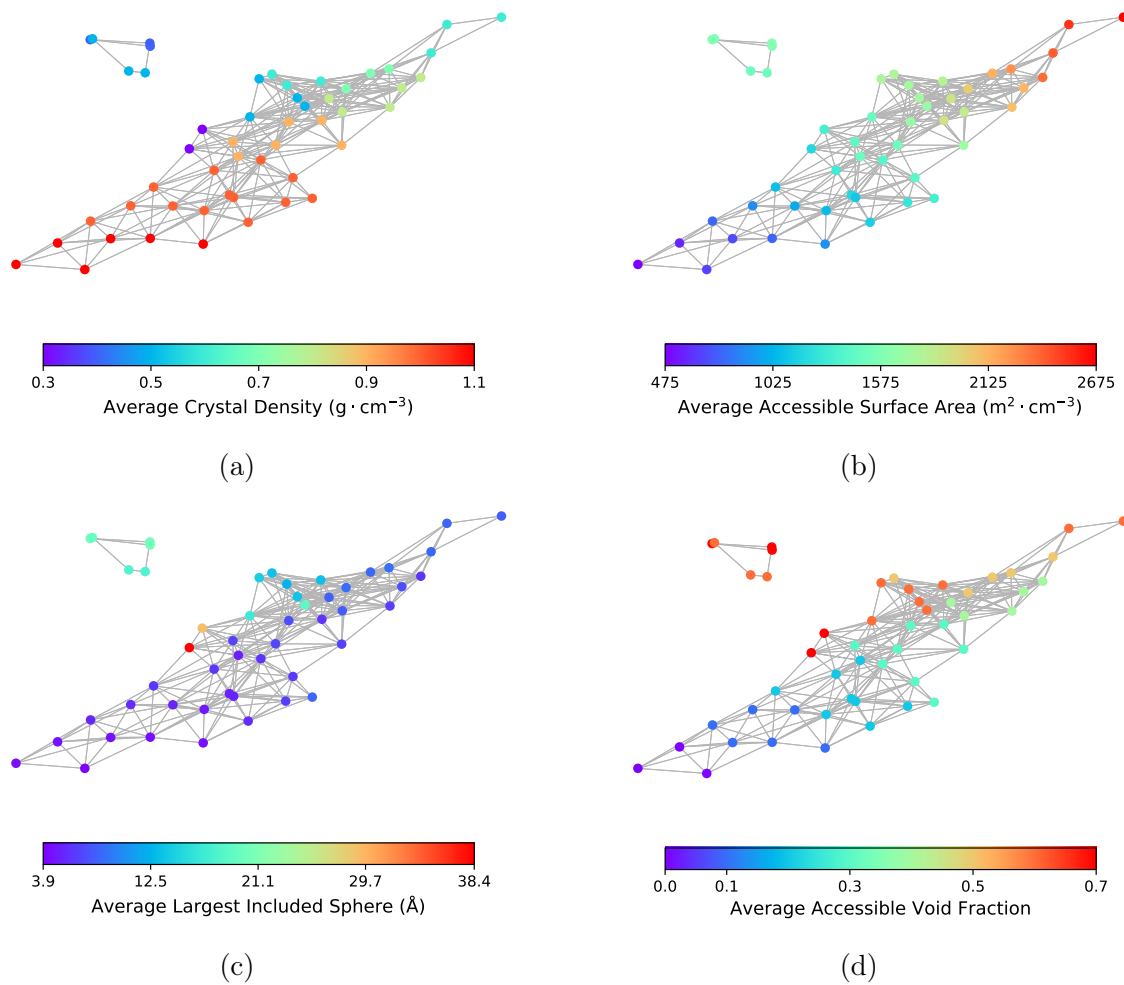
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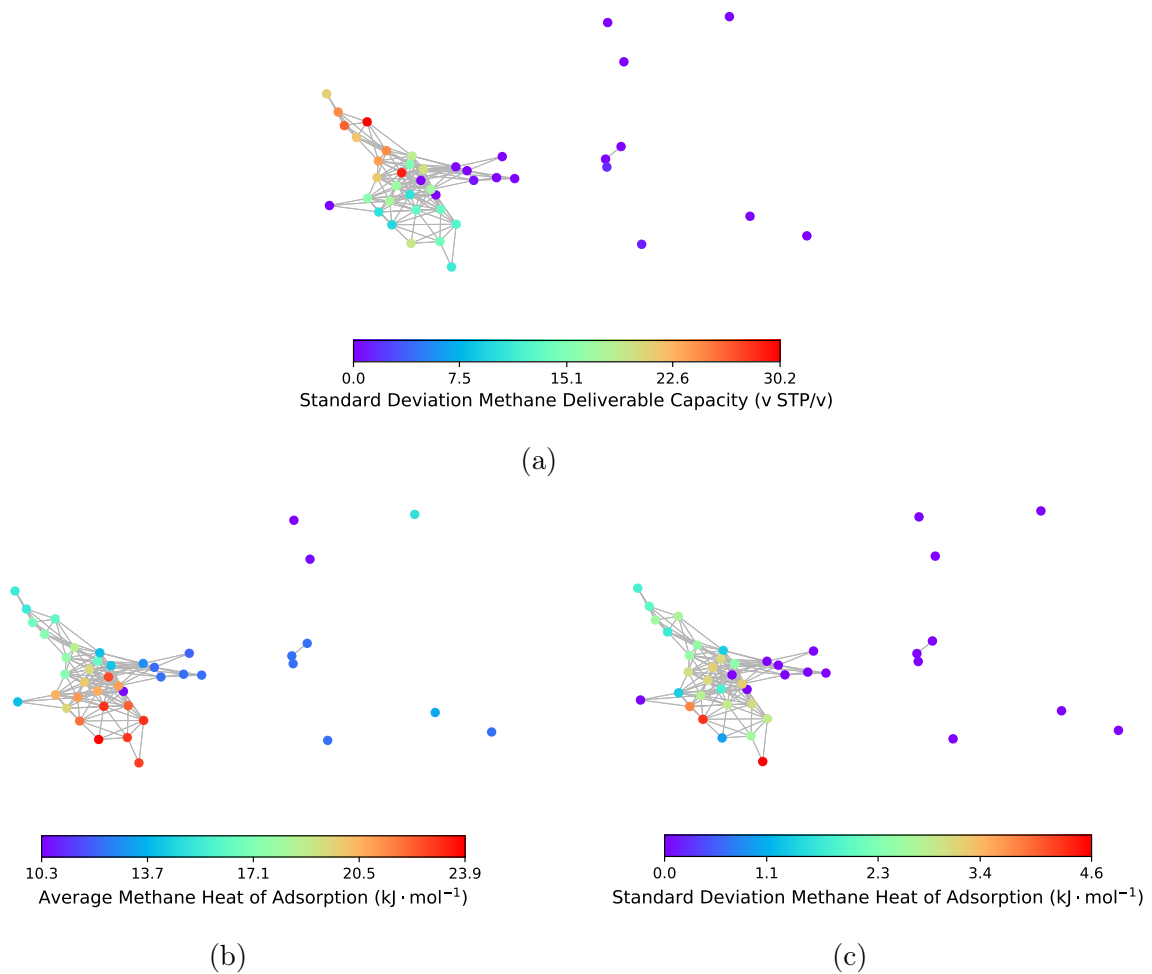
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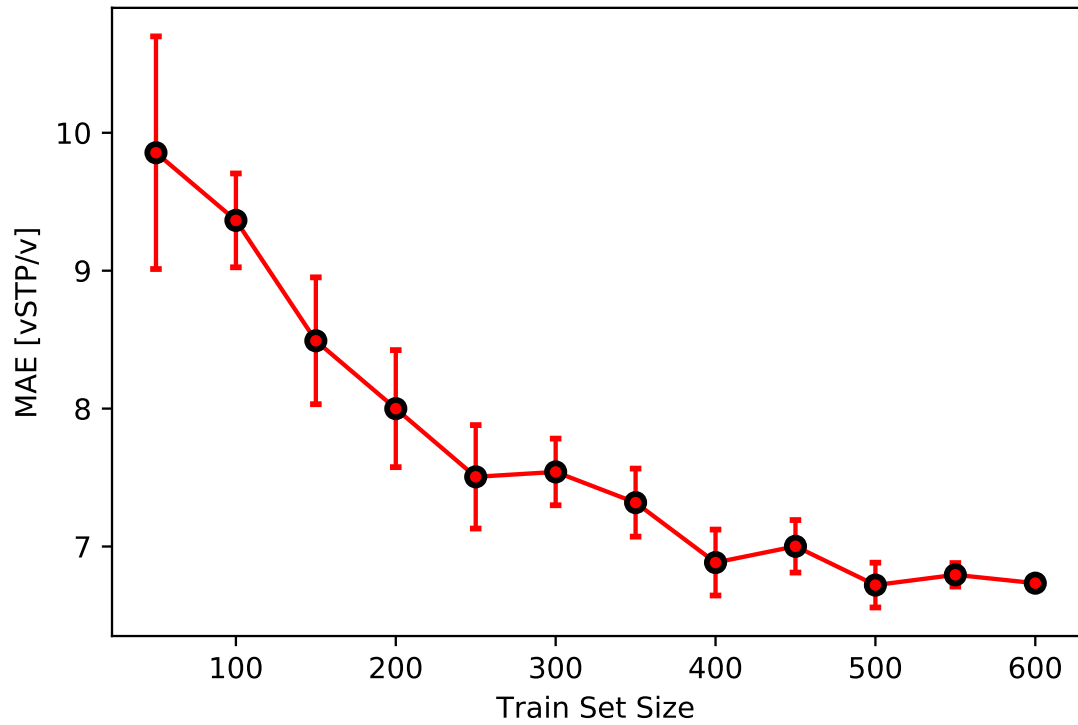
Supplementary Figure 1: The geometric landscape of **T0** molecule. The color coding shows the average conventional geometric descriptors, (a) crystal density, (b) accessible surface area, (c) largest included sphere, and (d) void fraction, respectively.



Supplementary Figure 2: The geometric landscape of **P2** molecule. The color coding shows the average conventional geometric descriptors, (a) crystal density, (b) accessible surface area, (c) largest included sphere, and (d) void fraction, respectively.



Supplementary Figure 3: The correlation between geometry and function for methane storage application for **T2** molecule. Low standard deviation in each bin of the geometric landscape shows the extend of importance of pore geometry for this application.



Supplementary Figure 4: Learning curve of the machine learning model. The mean absolute errors (MAE) were computed 10 times each with a unique random seed for each train set size. Error bars show the standard deviations.