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Entropy density and Mutual Information measures to quantify the complexity of a nanoscale system ILYA GRIGORENKO, VINCENT CRESPI, Penn State — Information-theoretic approach is the most general way to quantify complexity of nanoscale systems. In this study the entropy density and mutual information measures were used to identify the optimal interaction parameters between nanoparticles, which lead to the maximum geometric complexity of self-assembled nanostructures. A generalization of complexity measures at a finite temperature and for nonequilibrium systems is also presented. The developed theory can be used for efficient in silico design of new self-assembled nanostructures with a complex geometry not achievable before.

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