

# Confirming Classical Nucleation Theory with Novel Energy Landscape Methods

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Energy landscapes have been recognized as a powerful tool for deciphering the very nature of materials. They have already been used to understand glass relaxation, protein folding, and catalytic performance but a landscape has the potential to fully describe the kinetics and thermodynamics of any system or process. In order to enable this description for the purpose of relaxation and crystallization, we present a novel software created to map energy landscapes, energy landscapes of common glass-ceramic systems, and new fundamental insights into the crystallization of liquid systems. This is achieved by using a combination of statistical mechanics and classical nucleation theory to find an effective nucleation curve of the system  $\text{BaO} \cdot 2\text{SiO}_2$ . The nucleation curve predicted is found to be within 1 order of magnitude of the experimentally measured values. Further insights derived from the energy landscape will be discussed.