

# **On the Cauchy-Born approximation: at finite temperature and with Dilute Defects**

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## **ABSTRACT**

Constitutive relations play important roles in the study of particular materials. Either experiments or massive simulations were needed to get such material properties. In this talk, I will introduce our recent work on the efforts of effectively evaluating material constitutive relations. It can be considered as generalization of traditional Cauchy-Born approximation, which only works for perfect system at zero-temperature.