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Predicting Fracture Propensity in Amorphous Alumina from its Static Structure using MD and Machine Learning

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Predicting Fracture Propensity in Amorphous Alumina from its Static Structure using MD and Machine Learning

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Based on MD simulations and classification-based machine learning, we reveal that the propensity of amorphous Al_2O_3 to exhibit nanoscale ductility is encoded in its static (non-strained) structure. The machine learning based softness metric trained from the spontaneous dynamics of the system under zero strain is able to readily predict its fracture behavior.

Reference: Du T., Liu H., Tang L., Sørensen S. S., Bauchy M., Smedskjaer M. M. Predicting Fracture Propensity in Amorphous Alumina from Its Static Structure Using Machine Learning. *ACS Nano* **15**, 17705-17716 (2021).