Two-Level States in Substitutional Mixed Crystal: Ab Initio Predictions for Glass Transitions

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The nature of glass transitions has been a subject of great interest in solid state community due to their universal characteristics ccurring for a large range of materials. Among many explanations for the origin of this universality, the two-level states (TLS) theory [1, 2] stands as the simplest but most successful one. However, the identities of the two-level states have been confirmed for only few systems, and even so, only at the level of molecular dynamic simulation, due to a large computational cost of *ab initio* calculations.

Here we presents an ab initio investigation for the nature of the two-level states in one of the substitutional mixed crystals observed experimentally to be a glassy material [3] , Ba_{1-x} Ca_xF_2. We determine the underlying mechanism of the formation of the two-level states, which is the symmetry breaking in crystal structure driven by chemically induced local strains. A modulated Landau theory reproduces all the *ab initio* simulation results, and leads us to a prediction for the spectral density of states in very good agreement with the experiment.

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[2] W. A. Phillips, Rep. Prog. Phys. **50**, 1657 (1987).

[3] J. P. Wrubel *et al.*, Phys. Rev. Lett. **96**, 235503 (2006).

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